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Conceptual Design Report

Steve Peggs, Editor





ESS Conceptual Design Report



Editor: S. Peggs.

Contributors: K. Andersen, D. Argyriou, K. Batkov, C. Böhme, S. Bousson, I. Bustinduy, C. Carlile, P. Carlsson, L. Celona, M. Comunian, H. Danared, C. Darve, P. Deen, M. Dell'Anno Boulton, R. De Prisco, G. Devanz, R. Duperrier, D. Ene, M. Eshraqi, S. Gammino, M. Göhran, S. Gysin, H. Hahn, R. Hall-Wilton, H. Hassan, K. Hedin, W. Hees, P. Henry, A. Hiess, A. Jackson, P. Jacobsson, A. Jansson, A.J. Johansson, C. Kharoua, O. Kirstein, E. Laface, G. Lanfranco, R. Linander, M. Lindroos, S. Molloy, J. Malovrh, D. McGinnis, F. Mezei, P. Nilsson, E. Noah, E. Oksanen, C. Oyon, S. Pape-Møller, T. Parker, J. Persson, S. Petersson Årsköld, F. Plewinski, B. Pottin, A. Ponton, P. Radahl, K. Rathsman, M. Rescic, T. Rod, R. Ruber, P. Sabbagh, R. Seviour, S. Skelboe, A. Steuwer, J. Stovall, M. Strobl, A. Takibayev, L. Tchelidze, A. Tibbelin, G. Trahern, H. Wacklin, L. Zanini, R. Zeng.

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Executive Summary

The high intensity spallation neutron source ESS is well set to start construction in 2013 and to deliver first neutrons in 2019. The project itself has been 20 years in gestation but there has been a determination amongst the user community and those working in national and international neutron laboratories in Europe that it would be built. That determination is what has brought the project in where it is today. The baseline specification is for a 5 MW power, long pulse facility delivering neutrons to 22 independent instruments for the study of materials in all their diversity from pharmaceuticals and membranes, to colloids and polymers, to magnetic and superconducting materials, and on to engineering and archeological artefacts. The user community is rich and equally diverse, containing approximately 6000 individuals according to figures produced by ENSA, the European Neutron Scattering Association.

This Conceptual Design Report represents the work of about 250 individual scientists and engineers around Europe and the rest of the world, with about 100 of them located in the central team in Lund in southern Scandinavia where the facility is to be built, with Sweden and Denmark as co-hosts. As this team has grown over the past 2 years, the work intensity and output has risen considerably. It has taken some time for the realisation that ESS is finally to be built, to be fully digested, but it is clear now that this is indeed accepted.

The CDR is a technical document. It does not address organisational matters, nor governance matters and less so financial matters, although it must be emphasised that these subjects are borne in mind in arriving at the scope of ESS and hence the specification of the facility.

Over the next 12 months, work will be engaged upon which will result in a Technical Design Report being produced together with a series of other documents such as an updated Costing Report. These documents will demonstrate the sound foundation upon which the project is to be constructed and are a necessary, but not sufficient, achievement to lead on seamlessly to construction. Sufficiency would require our 17 partner countries to reach a political and financial agreement. We are confident that it is within their capabilities and resources to do so, and we look to them for such a signal.

I wish to thank Steve Peggs as editor and the whole team behind this work for their dedicated and wholehearted commitment.

Colin Carlile Director General European Spallation Source February 2012

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1 Introduction

1.1 The evolving story

The road for achieving a high power spallation source for Europe has been long and winding, with many twists and turns, but always with a determination to succeed. The production of this Conceptual Design Report is a concrete demonstration of the positive manner in which this project, long in gestation, is now maturing. Europe is working together in order to build, in southern Scandinavia, a slow neutron source of unparalleled power and scientific performance.

Let us look briefly at the history of the project. Neutron scattering, as a tool for the investigation of materials in all their diversity and complexity, was pioneered in the north American sub-continent in the 1950s. The first sources of neutron beams, as shown in Table 1, were extracted from the early research reactors that were constructed in a number of national laboratories in the USA as well as in Canada. It was on these research installations that the early instrumental techniques using neutrons were developed in order to begin to unravel the atomic structures of relatively simple materials and, uniquely, the atomic dynamics of these same materials. For this work Cliff Shull and Bert Brockhouse were awarded the Nobel prize in physics in 1994, many years after their pioneering work but at a time when the power of neutron beams to investigate the very wide spectrum of materials upon which much of our daily lives depend had been well and truly demonstrated.

Facility	Location	Status	First	Power	Instruments	Integrated	Peak
			oper.			$[10^{14} \text{cm}^{-2}]$	$[10^{15} \mathrm{cm}^{-2} \mathrm{s}^{-1}]$
ESS	Lund	Pre-constr.	2019	5	22	_	40
J-PARC	Tokai	Re-furbish	2009			_	
SNS	Oak Ridge	Operating	2006	1	14	_	
ISIS	Oxford	Operating	1984	0.2	27	_	4.5
SINQ	Villigen	Operating	1996	1	15	1.5	
IBR-II	Dubna	Re-furbish.	1977	2		0.1	10
PIK	St. Petersburg	Construct	_	100		40	
CRR-II	Beijing	Operating	2010	60		8	
ARR-III	Sydney	Operating	2006	20		2	
FRM-II	Munich	Operating	2004	20	24 + 6	8	
JRR-III	Tokai	Operating	1990	20	34	2.7	
RSG	Serpong	Operating	1987	30		2.5	
Dhruva	Mumbai	Operating	1985	100		1.8	
BER-II	Berlin	Operating	1984	10	16 + 3	1.2	
LLB	Saclay	Operating	1980	14	22 + 3	3	
ILL	Grenoble	Operating	1971	58	27 + 10	13	
NIST	Washington	Operating	1967	20		4	
HFIR	Oak Ridge	Operating	1965	85	11	26	
LVR	Rez	Operating	1957	10		1.5	

Table 1: The European Spallation Source in comparison to other high-level neutron sources that are operating, or are close to operation.

As with all new technologies there was a rapid rise in capabilities over the following two decades that culminated, in the late 1960s, in the construction in Grenoble in south eastern France of a purpose-built high flux reactor source of slow neutrons which was rapidly to become the focus of world attention and scientific endeavour in this discipline. Building upon the global effort in instrumentation, the Institut Laue Langevin, as it was named, became the flagship of neutron research and an exemplary demonstration of how two European countries could work together for the good of mankind. The ILL secured a scientific lead that, even 40 years later, it has retained and in many ways, consolidated.

In parallel, and with a somewhat different purpose, accelerator-driven sources of neutrons were also being developed. These facilities were excellent generators of fast neutrons that were used to great effect to compile a nuclear cross-section database of all the elements and their isotopes in order to support the nuclear power industry. These sources were pulsed in nature with a very high peak brightness. It was realised rather early on that such accelerator-driven sources held out significant opportunities for neutron technologies, provided that some of the disadvantages could be overcome. The early such sources were based on electron linear accelerators that had significant background problems caused by the very intense gamma radiation bursts which were generated. Nevertheless the opportunities for neutron scattering investigations were demonstrated with these early machines which were built around the world. These machines produced their beams of neutrons as sharp pulses, unlike the research reactors that produced continuous beams. Each type of source has its own rather unique characteristics that can be harnessed for the study of materials. The complementarity evident then still exists today.

At about this time – the late 1970s and early 1980s – the use of proton-driven neutron sources, either generated by cyclotrons or synchrotrons or linear accelerators, was beginning to be explored. Proton sources do not suffer from the gamma background which electron sources suffer from and the fundamental disadvantages of the earlier machines were overcome. Pioneering work at Argonne National Laboratory and Los Alamos National Laboratory in the USA and in Tsukuba in Japan indicated that pulsed proton sources held out a significant technological advantage over the most intense research reactors. This was because the spallation reaction employed in proton machines generates significantly less heat per useful neutron than does a fission reactor. In addition the generation of neutrons in pulses provides peak brightnesses which far exceed those available from reactors.

The enthusiasm for such proton machines led to ambitious conceptual designs for neutron sources that went well beyond the technological capabilities of the time. Far-sighted projects such as the ING source in Canada, the SNQ project in Germany and the pulsed reactor SORA of the European Community were planned. None of these was ever built but they provided the seeds from which the European spallation source has grown.

In the early 1980s, the construction of the world's first proton spallation source which was powerful enough to challenge the supremacy of the ILL was started. It was a pioneering endeavour that had many doubters but which succeeded, over a difficult decade, both in achieving its design specification and to completely overturn the accepted wisdom. This source, built close to Oxford in the UK, was called ISIS. Despite having a power of less than 200 kW it demonstrated quite clearly that world-class science could be carried out very effectively on such sources. ISIS was the birthplace of many new instrument concepts, some of which had been prototyped on other neutron sources. ISIS also provided a degree of support to the user community that went beyond the currently accepted relationship between the central facility and its user community.

The next chapter in this story sees the OECD Megascience Forum producing a study of the future evolution and needs for neutron beams in a global context. This study took place in the early 1990s and resulted in a report to the research ministers of the OECD countries which recommended that a megawatt-class spallation neutron source be built in each of the three developed regions of the world.

Europe in the late 1990s was in an enviable position in this scientific field. It not only had what were unquestionably the world's leading reactor source of neutrons and the world's leading accelerator-based source of neutrons, but it was blessed with a network of medium and low intensity neutron sources which were breeding grounds for innovative instrumentation and the origin of new scientific ideas. Accordingly, the community of researchers in Europe who used neutrons for a significant part of their scientific research programme, grew rather spectacularly both in numbers and in diversity. The figure today, according to a survey made by the European Neutron Scattering Association, sits at around 6000 individuals. It was therefore a completely logical step that many of these scientists started to lay down plans for the European facility which had been foreshadowed in the OECD recommendation. An international task force was assembled, originating from perhaps 20 countries, which began the task of defining the scientific case for such a facility and designing the source which was capable of delivering this scientific goal. This resulted in a 2002 design study for a 10 MW spallation source with two targets and furnished with more than 40 neutron instruments which was powered, not by a proton accelerator, but rather by an H-minus accelerator, the beams from which could be injected into a compressor ring and compressed in time to less than 1 μ s in duration. By this time the United States and Japan had both begun the construction of megawatt capacity spallation neutron sources, both of which are now operational.

Europe however, furnished with its rich network of neutron sources, collectively allowed itself a more relaxed procedure which has, in the long-run, been beneficial, even though at that time this slowness in decision-making was not universally appreciated. This ongoing study on the ESS resulted in a comprehensive set of documents laying down the scientific case for the ESS being produced, together with extensive technical documentation and costings [1, 2, 3, 4, 5]. These studies were presented to a plenary meeting of ESS stakeholders in May 2002 in Bonn attended by more than 700 scientists and science policy-makers. Although this meeting was a very positive endorsement of the use of neutrons for materials science and was excellently organised, in retrospect it proved to be the beginning of a reshaping of the whole project that created an opportunity for sites other than those in Germany and Britain to consider bidding for the location of ESS. In 2003, a new concept was put forward for the ESS that involved descoping the whole facility and a fundamental change of technical orientation. The new design comprised a proton linear accelerator delivering a 5 MW long pulse to a single target station surrounded by a suite of 20 to 25 neutron instruments. The H-minus beam, the compressor ring, the second target station and the constrained moderator configuration were all abandoned. This initiative held out the

promise of neutron intensities that were a factor of six more intense, per megawatt of proton beam power, than currently existing facilities.

It is this concept from 2003, which was endorsed by the user community in Europe and which is now the subject of the ESS Pre-construction Phase currently underway, which will deliver first neutrons in 2019. The Pre-construction Phase contains within it a complete Design Update, a totally revised cost estimate and time-schedule, and the beginning of a Prepare to Build project that prototypes key components in order to minimise technical risk during the construction phase that will commence in 2013.

In the intervening years from 2003 to 2009, a number of significant steps were taken. Three sites emerged as contenders for the location of ESS. These were Debrecen in eastern Hungary, Bilbao in northern Spain, and Lund in southern Sweden. The three site contenders worked both competitively and collaboratively in an intense process which led, via the European Strategy Forum for Research Infrastructures (ESFRI) and ultimately overseen by the Czech research ministry during its period as president of the European union, to the selection of Lund in Scandinavia as the preferred site. This choice followed a site review process during the summer of 2008 that resulted in a report presented to the major ESS stakeholders in September of that year. In Brussels on the evening of May 28, 2009 a decision on the site was arrived at.

Thereafter, following further negotiations, Spain and then Hungary endorsed the choice of Lund. The team in Lund had been administered within Lund University as a special entity and funded by Scandinavian organisations. With the site decision, a new governance of the growing organisation, with its important tasks to fulfil, was put in place. Two lines of governance were created – firstly the more standard Steering Committee with representatives from the various partner countries, and a legal Board which represented the formal owners of the project which were, for administrative and legal purposes, Sweden and Denmark who were co-hosts and therefore co-owners of the emerging facility.

At the time of writing – December 2011 – ESS AB is a shareholding company under Swedish law with Sweden holding approximately 75% of the shares and Denmark holding the remaining 25%. The Steering Committee has now 17 partner countries¹. Various advisory committees are active to advise the governing bodies and the ESS company.

The 17-partner international collaboration was signalled by the signing in Paris at the Swedish Embassy of a Memorandum of Understanding on 3rd February 2011. This MOU was a non-binding agreement that nevertheless contained three guiding principles. These were an acceptance of Lund as the site for the ESS, an agreement to engage in and to proceed with the Design Update of the ESS and, thirdly, to make best efforts to continue on to the construction phase in a timely manner.

This present Conceptual Design Report represents the technical work carried out during the 12 months between signing of the MOU and its first anniversary. It will be followed by a Technical Design Report which will be delivered prior to the second anniversary of the signing of the MoU on 3rd February 2013.

The current work programme contains three separate streams: the Design Update and revised costing activities; the start of the Prepare to Build phase, which involves the prototyping of key equipment in order to minimise future risk; and the necessary work for integration and acceptance of the project by its stakeholders within Europe and more locally.

¹Sweden, Denmark, Norway, Latvia, Lithuania, Estonia, Iceland, Poland, Germany, France, the United Kingdom, the Netherlands, Hungary, the Czech Republic, Switzerland, Spain, and Italy.

1.2 Top level parameters

Table 2 records the High Level parameters of the ESS, and its guiding scientific goals. The starting point for the generation of these parameters was the 2008 ESFRI Roadmap specification. The parameters shown were updated and approved on April 18, 2011.

Parameter	Unit	Value
Average beam power	MW	5
Number of target stations		1
Number of instruments in construction budget		22
Maximum number of instruments		44
Number of beam ports		50
Number of moderators		2
Separation of ports in degrees	0	5
Proton kinetic energy	GeV	2.5
Average macro-pulse current	mA	50
Macro-pulse length	\mathbf{ms}	2.86
Pulse repetition rate	Hz	14
Maximum accelerating cavity surface field	MV/m	40
Maximum linac length (without 100 m upgrade space)	m	482.5
Annual operating period	h	5200
Reliability	%	95

Table 2: High Level parameters, April 18, 2011.

Performance

- Neutron production 30 times SNS today.
- Peak neutron flux 30 times ILL's average flux.
- Time-averaged neutron flux equal to ILL.
- Electrical power supply 32 MW to 38 MW.

Target

- A single target station furnished with cold and cold-thermal moderators.
- A solid rotating tungsten target.
- A liquid metal target as reference for licensing purposes.

1.3 The ESS programme

The ESS programme is now well into its Pre-construction Phase, following the timeline shown in Figure 1. The programme contains within it three project lines:

- 1. Design Update.
- 2. Prepare to Build.
- 3. Construction and Operations.



Figure 1: Master programme schedule, showing the *Design Update*, *Prepare to Build*, and *Construction and Operations* project phases.

The third project is ongoing and continuous and will remain an important element throughout the whole lifetime of the ESS facility. Basically it is an information activity maintaining effective dialogue with our major stakeholders be they scientists, politicians, funders, laypeople, et cetera, and be they local, regional, national or international in origin. The activities involve both the traditional media and the rapidly evolving e-media. In real terms this encompasses press releases, web pages, talks, visits, exhibitions, branding, brochures, annual reports and one-to-one interactions. We have built up a strong communications culture and this is to be constantly updated, appropriate, attractive and relevant.

It is very important that the project has many supporters, but it is perhaps even more important that it has few enemies. Public acceptance is crucial to success and we put particular effort into this.

The second element above – Prepare to Build (P2B) – is a project where key elements of the whole facility are prototyped in order to minimise the risks during construction and to ensure high reliability during operations. The P2B phase will extend well into the construction phase and, indeed, any item where prior development is necessary before committing constructional funds should, in general, be prototyped. For practical purposes we see the P2B as extending to 2016.

The first item – the Design Update (DU) – is the project that carries the highest combination of urgency and importance. It is, to a great extent, the major topic of this Conceptual Design Report. The DU is an exercise in conception, design, computation and, critically, project organisation. It will deliver a design for the whole facility, not, in many cases, a ready-for-procurement design. Detailed design will be an ongoing activity utilising resources as and when necessary and not prematurely but timed so as to ensure procurement, manufacture and

Parameter	Unit	Value
Capital cost criterion	В€	1.5 maximum
		Audit in-kind contributions
		Ring-fence budgets at level 2
Timeframe for construction		2013 to 2018
Commissioning and completion		2019 to 2024
Operations		2019 onwards
Annual operating cost	М€/у	103

Table 3: Cost and timeframe parameters.

delivery on time and not significantly, ahead of time. A central part of this process will be an updated time plan and an updated costing report indexed to 2013 values.

In the meantime we work with our current time plan which indicates first protons to the actual target in 2019 – and hence first neutrons to the Day One instrument suite of seven instruments – and full specification being reached in 2025 with the accelerator operating at 5 MW proton power, 22 separate neutron scattering instruments taking data and a healthy but still growing neutron user community generating top-class science. Equally well we are working on the budget as defined in the 2011 comprehensive Costing Report [6] which indicates a total capital cost for the facility complete with its 22 instruments of 1,479 M \in in January 2008 values. The current cost and timeframe parameters are shown in Table 3. All options for upgradeability are to be examined with associated additional contingent costs up to a pre-determined limit of the capital cost and to be authorised by the governing bodies.

With 17 European partners committed to construct ESS, it is inevitable that a significant source of revenue will be components manufactured and supplied as in-kind contributions. For planning purposes the ESS organisation has the expectation that 75% of the capital cost will be cash contributions and that 25% will be in-kind. Currently representatives appointed by the Swedish and Danish governments are engaged in bilateral discussions with the other partners in order to determine the potential of each country to engage in the construction process starting in 2013 and at what level.



Figure 2: Programme organisation and governance organigramme.

The significant fraction of in-kind contributions brings with it particular challenges. The optimal and ideal solution of 100% cash to a central project team is not attainable and therefore management of in-kind contributions is the key issue in delivering the ESS on time, to budget and fully operational. The technical

risks of managing interfaces need special attention and, indeed, additional resources will be required to do this effectively. 100 M \in is not an unrealistic additional sum for this purpose.

The governance of ESS is illustrated diagrammatically in Figure 2. It is complex and it is clear that this must be simplified at the earliest opportunity. Legally and administratively ESS reports to a governing Board populated by Swedish and Danish members reflecting the 3:1 shareholding of the two countries and their status as co-hosts. A Steering Committee, which gathers together delegates from the 17 partner countries, also functions in parallel to the ESS AB Board. The STC is a more traditional governing body, being populated by scientists with experience of large scientific infrastructures together with ministerial or research council personnel who are close to the funding authorities from their individual countries. The STC is aided in its job by an Administrative and Finance Committee, which is formally a sub-committee of the STC, populated by national delegates. Two further advisory committees exist which are directly related to the ESS organisation itself and are the source of independent advice. These are the Scientific and Technical Advisory Committees respectively. They are populated by international scientific and technical experts and are nominated by the ESS Company itself. They do not map onto the 17 ESS partner countries.

The ESS Company itself is in a rapid growth phase. This requires careful guidance and management. Currently we are close to 100 people organised into five managerial groupings. The Director General's services represent the smallest, comprising communications and special advisors. The four Directorates, each headed by a Director, are Accelerator and Target, Instrument and Science, Administration, and the ESS Programme Office. The organisation operates on a customer-supplier basis managed by the ESS Management Team (EMT), which the Director General chairs. Technical authority rests with the ESS Programme Group, chaired by the Programme Director and attended by all Directors. The architecture of authority and responsibility is not organised in a vertical hierarchical structure but rather is built on a strong team with distributed authority and responsibility. The organisation is significantly flatter than equivalent organisations set up in the second half of the 20th century, with which we are often compared. It is run in a collegiate spirit rather than in an authoritative one.

2 Neutron Science

2.1 Scientific drivers

2.1.1 Man as materialist

Throughout the ages, man has been a materialist. Indeed, the ages of human development – the stone, bronze and iron ages – were named directly from the materials that mankind used to advance itself through the different stages of civilisation. These advances in materials did not stop after the iron age, as shown in Figure 3, quite the opposite. Materials have enabled human development up to the present day and will continue to define our various stages of development and achievement as a species in the future.



Figure 3: The materials used by man have defined the stages of civilisation.

Many modern materials developed from ancient metallurgy, after the availability of ceramics enabled ores to be smelted. Over time we learned to make stronger metal alloys and tougher ceramics, mostly via a trialand-error process. For example, Damascus steel swords reaped fame in the middle ages for their toughness and resistance to shattering. But back then there were no probes to examine microstructure, nor were there quantitative ways to test for toughness or yield strength. While the nature of matter has been debated since the time of Democritus, who postulated the existence of atoms, it was the advent of thermodynamics in the 19th century that offered us the concept of a "phase" and hinted that the properties of materials are dependent on the arrangements and motions of the atoms that constitute them. The means to probe the atomic structure of materials was not realised until the work of Röntgen, von Laue and Bragg provided the X-ray tools and the means to interpret these data from crystalline materials. Indeed, the early work of X-ray diffraction progressed from establishing the crystalline structure of salts and into the toughest of problems at the time: the structure of DNA.

While X-rays have been used extensively to investigate materials, the emerging nuclear age of the 20th century offered new opportunities. In 1932 Chadwick discovered the neutron, which can be produced in substantial amounts inside the core of nuclear reactors. The work of Cliff Shull and Bert Brockhouse demonstrated that neutrons can diffract just as easily as X-rays, and can report not only on crystal structure but also on magnetic structure, as well as monitor the dynamics of atoms and magnetic pinning in crystals. For the first time, we were in a position to obtain a complete picture of why the properties of materials differ so much on an atomic scale. Indeed, the early achievements of neutron science were the confirmation of anti-ferromagnetism predicted by Louis Néel and quantised lattice and magnetic excitations known as phonons and magnons, demonstrating that neutron scattering is a valuable probe in understanding materials and their properties, and facilitating significant progress in scientific understanding. Today, neutrons from both reactor and spallation sources are used widely to understand the nature of the solid and liquid states of matter, as an analytical tool to aid the development of materials for society and as a tool to examine curiosity-driven research that spans from cosmology to strange magnets, from superconductivity to the dynamics of the molecules of life.

2.1.2 Why do we need neutrons?

"If the neutron had not been discovered by Chadwick in 1932, it would have been invented." Bertram N. Brockhouse, Nobel Laureate in Physics 1994.

The use of neutron scattering as an analytical technique was developed in the second half of the 20th century. As technology and theoretical understanding have improved, it has evolved into a diverse range of powerful methods capable of extracting very subtle information about the properties and behaviour of many different kinds of materials. Europe has been particularly strong, providing a range of facilities for a large and increasing number of scientists that use the technique. Neutrons offer many advantages as a probe to study matter as well as the fundamental premises of Nature itself. While the most important benefits are described in the list on the next page, it is noting that neutron scattering methods are highly complementary to the X-ray methods available at dedicated light sources (synchrotron facilities). Indeed, both are frequently used in parallel to solve the most difficult of problems in many areas of science and technology.

The ESS will offer neutron beams of a brightness unparalleled by what has been achieved before in dedicated neutron sources: five times more powerful than any other spallation source and 30 times brighter that the world's most powerful reactor-based neutron source. To achieve this performance, the ESS will use new technology and novel approaches in neutron scattering. Due to the novelty of the technology, the longer, brighter neutron pulses of the ESS bring unique opportunities to the design of appropriate neutron scattering instrumentation. These opportunities will be exploited by calling on the experience of instrument designers in Europe, on both pulsed and continuous sources. The instrument developers and scientists in the community have already begun to take advantage of these opportunities, capitalising on recent advances in neutron optics and instrument design. The key question for the scientific community now is how to use the brightest neutron pulses in the world. Which are the key areas of science that will benefit most from the bright ESS beams, and how do we best prepare to address them? Predicting the future frontiers of science is a precarious endeavour, but it is clear that neutrons can directly address some of the grand scientific and technical challenges that face our society today.

Six good reasons for using neutrons.

- 1. A wide range of length and timescales. Neutron scattering enables scientists to study the structure and dynamics of atoms and molecules over an enormous range of distances and times, from a micron to one-hundred-thousandth of a micron, and from a millisecond to ten-million-millionths of a millisecond. While other techniques can provide information either within the same distance range or the same time range, this combination of both structural and dynamical information is unique to neutrons.
- 2. An ideal probe for magnetism. The neutron acts as a tiny magnet, but has no charge, so we can use it to study the magnetic structures and dynamics of materials at the atomic scale. This magnetic behaviour is the basis of many common devices, such as computer hard disks.
- 3. High sensitivity and selectivity. Neutrons are scattered by atomic nuclei; the degree of scattering depends not only on the element but also on the specific isotope. Elements of similar atomic weight, or different isotopes of the same element (such as hydrogen and deuterium), can scatter quite differently. This introduces the possibility of substituting one isotope for another (by clever chemistry or biotechnology) to highlight particular groups of atoms in mixtures or complex materials. Of particular importance is the fact that neutrons are very sensitive to both hydrogen and deuterium. This has led to a powerful method using selective deuterium substitution to study complex biological and other hydrogen-containing materials, especially those containing water.
- 4. **Deep penetration.** Neutrons pass easily through most materials, allowing the study of large or bulk samples, and buried interfaces, or materials under extreme conditions such as high temperature or pressure. Neutrons are nondestructive, so delicate materials or precious objects can be studied without fear of damage. Neutron imaging can be used to "look inside" objects as large and complex as an operating car engine.

- 5. A probe of fundamental properties. Studies of nuclear and particle physics using neutrons can probe the building blocks of Nature, helping us to understand events from the creation of the fundamental particles and forces during the first fractions of a second after the Big Bang, to the explosions of massive stars, such as supernovae, in which most of the heavier elements were created.
- 6. A precise tool. Neutrons are an extremely precise tool. Their interaction with atoms is not very strong, which makes analysing the data, and understanding it, straightforward. We can easily compare neutron scattering results with computer simulations or models. Slow neutrons, which carry low energies, are not damaging to sensitive samples.



Figure 4: Research using neutrons covers many disciplines, holding potential for fundamental science as well as new applications.

2.1.3 Science using neutrons – today and tomorrow

The span of possibilities for the ESS is as broad as science itself. Neutron scattering can be applied to a range of scientific questions, spanning the realms of physics, chemistry, geology, biology and medicine. With a neutron tool kit, we can probe the molecular basis of health, biology and the life sciences. We can obtain a deeper understanding of the fundamental aspects of matter and what makes different materials behave the way they do macroscopically, and we can dive down and conduct fundamental studies of the neutron itself. Furthermore, neutron imaging techniques enable investigations of fossils and artefacts, thus bringing neutron science into the realm of the humanities and heritage studies. Clearly, the scientific areas overlap and interact, erasing the traditional academic boundaries in the quest for knowledge. Our quest for understanding the molecular and atomic interactions that define the world in which we live spills over as innovations and applications for humankind. Solutions for a sustainable, healthy and technologically empowered society arise from scientific curiosity, just as dedicated development of improved applications leads humanity to new discoveries, as illustrated in Figure 4. This is as true now as it was in the time of Damascus' steel swords. Science and innovation go hand in hand in an unpredictable fashion and, as our understanding of the world increases, we will move on into the future equipped with hitherto unknown materials and insights.

A selection of successful front-line research endeavours is presented below, explaining how neutron science has enabled developments and highlighting the potential that the superior capabilities of the ESS bring to each project. **High-performance alloys.** Human progress has been driven by the availability of new materials with useful properties, from the first metals extracted from ores, through ceramics and glass, to the plastics and composites of today. The goal now is to design novel materials whose function relies on complexity that is tailored and built in at the atomic level. Neutrons provide a unique set of tools to probe their structure and performance over a wide range of length and timescales. As early as 3000 BC, people discovered that melting copper and tin together made an alloy, bronze, which is more durable than its components. Over the past century, a wide range of alloys has been developed. Many are lightweight, high-strength materials composed of metals and other elements not available to our ancestors. Advances in metallurgical research have given us a good understanding of the behaviour of alloys on different length scales, as the structure at the atomic level strongly determines the performance of the bulk material.

Neutron scattering techniques have played a significant part in this development, due to the ability of neutron beams to penetrate deep inside complex equipment used for controlling the temperature of the materials under study. They have, for example, allowed researchers to find the optimal heat treatment to grow alloys with a controlled crystal structure that maximises their performance. This has led to the development of alloys such as high-strength aluminium and titanium, used to make cars and aircraft lighter, skyscrapers stronger and laptop cases stiffer. Although the research may be driven by the needs of the defence and aerospace industries, the technology is often transferred into consumer areas: racing bike frames are made of the same tough aluminium alloy as aircraft wings, and hip replacement implants use the titanium alloy employed in the manufacture of aero-engine turbine blades. The number of possible chemical combinations of different elements that can be incorporated in an alloy is vast, and we have explored only a small fraction. For example, novel alloys with complex crystal phases, such as transformation-induced plasticity (TRIP) steels, which combine high strength and formability, are being developed for use in the automotive industry. Another new ultra-hard steel, super-bainite, is designed for armour plating. Neutron scattering will remain an essential tool required for characterising such materials for many decades to come.

Green energy with novel fuel cells. Producing and consuming energy is the main cause of the environmental problems that the world is facing today. New, advanced materials for greener power generation schemes such as solar cells, fuel cells and batteries are pivotal for a smooth transition to a society built on sustainable energy production. Despite intense R&D over the past two decades, fuel cell technology is still not ready for large scale commercialisation. In low temperature fuel cells, which would be the primary choice for the transport sector and consumer electronics, the proton exchange membrane fuel cell (PEMFC) is currently the preferred technology. PEMFC development is being held back by the limited performance of the polymer membranes currently available, and also by the cost and efficiency of the electrode catalyst. Research is thus focused on developing new membrane materials, as well as understanding the catalytic mechanism to improve efficiency. Neutron scattering techniques are used to monitor the movement of hydrogen ions across the membrane and their interactions with the electrode. Since new membrane materials are complex composites, revealing their structure and following the dynamic processes within them requires high-intensity neutron beams as offered by the ESS. In addition, the ESS will enable *in situ* studies, which will allow us to follow the catalytic reactions kinetically and even image the whole fuel cell under working conditions.

Conserving energy with better batteries. The lithium battery has revolutionised consumer electronics. The widespread use of laptops and smart phones would not be possible without a battery providing a high discharge rate, long standby time and long cycle life. The lithium battery, with its high energy density, has exactly these characteristics. There is currently a huge research effort going into scaling up the technology for use in hybrid vehicles, as well as developing an energy storage device for wind farms and other renewable energy production schemes. The key to an efficient battery is the ability to store (intercalate) a high concentration of lithium ions in the electrodes and to transport them effectively through the electrolyte. The process also has to be reversible to generate a large number of charge/discharge cycles. In explorations of new battery materials, neutron scattering offers the unique advantage of distinguishing light atoms in a matrix of heavier elements. In addition, the deep penetration of neutrons allows for *in situ* studies. At present, research with neutron scattering has been carried out mainly on test-model systems. But with the high power of the ESS, researchers will be able to investigate more complex materials of commercial interest, and also monitor battery packs in real time while they are actually charging and discharging.

Green catalysts. Another important field, which leads to more efficient energy use as well as reduced environmental pollution, is the development of new catalysts. Catalysts are materials that speed up specific chemical reactions, often by lowering the temperature or pressure at which the reactions occur. They are essential to the manufacture of other materials such as plastics, pharmaceuticals, fuels and fertilisers. Also, catalysts are vital in controlling pollution from vehicles. Catalytic converters, which reduce carbon monoxide and nitrogen oxide

emissions, rely on a fine mesh of platinum-coated ceramic through which the exhaust gases pass. Chemists are continually looking for better catalysts that are more selective, more efficient and more environmentally friendly. The ideal catalyst should remain active over many reaction cycles and produce no side products. It should furthermore allow a reaction to occur in water rather than in an organic solvent (which is a source of pollution), at ambient temperatures and pressures and with little toxic waste. In this endeavour, neutronscattering techniques provide a unique tool in that they allow the study of active catalysts as they are working. Researchers can follow the individual steps of a catalytic process, and so optimise and tailor catalyst structure. Transient chemical species that form during the reaction can be identified by their crystal structure using neutron diffraction, or by studying how their characteristic vibrations change the neutron energy. Many reactions involve organic compounds containing hydrogen, which lend themselves to analysis by neutron methods.

Decoding the molecular basis of life. X-ray, electron microscopy and, increasingly, neutron studies of biological tissues have produced breathtaking pictures of cells, organelles and the molecular machines of proteins and nucleic acids. The morphology and behaviour of bio-molecular assemblies provide insight into the molecular basis of life – but also into the unwanted molecular developments that result in disease. An understanding of diseases such as cancer and diabetes is used in the design of new, more effective treatments. However, much is still unknown about how biological systems operate, both in health and in disease, at the sub-molecular level and at the scale of larger molecular assemblies. Whereas recent advances in structural biology have been dominated by X-ray scattering, neutron technology is now approaching levels of performance that can meet the difficulties associated with biological materials, such as the typically limited sample sizes available. This opens up a new vista of possibilities, as neutrons can monitor aspects of matter that are currently inaccessible to X-rays. The powerful complementarity of the two methods is predicted to solve major challenges within the life sciences. Recent advances in neutron spallation source technology will be fully exploited in the development of the ESS, providing the high flux necessary to meet the challenges presented by health and life sciences.

Beautiful DNA. The beautiful, ladder-like structure of DNA molecules wound into a double helix was first revealed by X-ray diffraction in 1953. This is one of the outstanding achievements in biology and it opened up a new era in our understanding of how genes regulate living processes at the molecular level. DNA consists of four chemical units (bases) arranged in long sequences called genes, each of which is responsible for making a particular protein in a cell. Biologists are now trying to elucidate exactly how DNA functions and interacts with other molecules to sustain life.

There are still many unresolved puzzles. For example, how can DNA be packed so tightly, in a virus for example, although when stretched out, it can be many microns long? Neutron scattering has successfully elucidated the structure and ordering of DNA in concentrated solutions, in particular in the presence of small ions, which can cause the DNA coils to collapse into condensed structures. Neutron diffraction has a broad application to the study of DNA fibres, as well as other biological fibres such as cellulose. Rather than assuming a globular structure (as with many proteins), these long chain molecules frequently assume a regular helical conformation leading to a fibrous state. Although these molecules might not necessarily crystallise, they can be aligned parallel to each other as fibres. Another important issue is how DNA binds water and other molecules, which can range from small drug molecules to large proteins. Neutron scattering is a powerful tool for investigating intricate DNA interactions. While the current focus is on structural investigations of complexes of DNA with other molecules, the ESS will offer superb time resolution, allowing researchers to follow structural rearrangements as they happen in these complex biological materials.

Probing proteins. A major milestone was reached in 2003 when the Human Genome Project – the international project to determine the full DNA sequence that makes up the 20,000 to 25,000 genes defining a human being – was completed. The even more comprehensive challenge is to identify the proteins coded for in the genome and to determine their structure, interactions and function. Proteins are the molecular machines that drive cells through their various life stages. Many are enzymes or receptors, mediating life sustaining processes such as energy conversion, cell division, immune responses and communications between cells; others have mechanical or structural functions. During the past 20 years, advances in X-ray crystallography have enabled molecular biologists to determine the 3-dimensional structures of proteins, which may comprise thousands of atoms, right down to the atomic level. While these protein maps have enabled advanced analysis of all kinds of biochemical and biophysical experiments and resulted in a much deeper level of understanding of biology at the molecular level, they also have some severe restrictions. Firstly, light atoms such as hydrogen are not easily discernible by X-rays. Secondly, crystallising membrane-associated proteins is very challenging, leaving this significant group of proteins (about 30% of the genome) underrepresented in terms of structural information. Thirdly, proteins in crystalline form do not necessarily represent their natural conformation(s), nor does the static crystal structure inform on the complex dynamics of biomolecules *in vivo*. The uniquely intense beams of the ESS, combined with recent advances in protein crystallography, will enable an increasing number of crystal structures to be solved by neutron diffraction. This will shed light upon light atoms such as the ubiquitous and pivotal protons – invisible to X-rays – addressing key questions such as how charge is moved across membranes, how water is oxidised to oxygen photosynthetically, how metabolic charge transfer reactions are catalysed, and how surface interactions cause proteins to fold in particular ways. For non-crystalline samples, the complementary methods of neutrons, X-rays, NMR and molecular dynamics simulations are well poised to bring structural biology to a new level. Using a combination of neutron scattering and molecular dynamics simulations, the dynamics of dissolved proteins and proteins in membranes will be addressed, hopefully shedding light on dynamic processes such as regulation, catalysis and signalling. The high intensities available at the ESS will also enable investigations of much smaller sample volumes than today. This creates potential for investigating a range of biologically and medically interesting samples available in limited amounts – such as materials from biopsies or other biological samples.

Treating cancer. Effective cancer chemotherapy requires that the drug be delivered directly to the tumour while avoiding healthy tissue. Several methods are being developed to target tumours selectively. One approach is to employ lipid vesicles, liposomes, which encapsulate the drug. Besides being highly biocompatible, liposomes offer the possibility of binding hydrophobic drugs on the interior face of the lipid membrane, or hydrophilic drugs in the internal aqueous compartment. "Homing" peptides, which recognise a cancer cell, can be attached on the outside of the liposome. On reaching the surroundings of the tumour, the drug is released by a mechanism such as heat (for skin tumours) or the specific chemical surroundings of tumours. Currently, much of the work in optimising these drug delivery systems focuses on the nanoscale structure of the liposome and how the drug penetrates the leaky barrier of tumour plasma membranes. Neutron scattering is a highly suitable technique for these investigations, especially as the drug and carrier components can be highlighted using deuterium substitution. Ideally, neutron experiments would be carried out on a live tumour to determine the efficiency of the targeting. This requires a small beam size, and thus a high intensity source such as the ESS.

New magneto-electric materials. Research into advanced materials for new types of electronic and electrical devices is a field of intense activity. These materials may have structures with novel electronic configurations, which combine more than one useful property. For instance, scientists would like to find a chemical compound that combines the property of ferroelectricity – in which the electric dipoles of atoms are aligned in one direction – with ferromagnetism, in which magnetic moments (the electron spins) are also aligned. Ferroelectric materials are used in actuators and sensors found in cars and planes, and as memories in digital cameras, while ferromagnetic materials are found everywhere from refrigerator magnets to read-write heads on computer hard drives. Combining the two effects introduces the possibility of controlling an electric field with a magnetic field and vice versa, opening up the potential for new, fast electronic switching devices and computer memories. For many years, it was thought that such a magneto-electric material was not possible. However, this conclusion was recently proven wrong.

The solution is to make use of a phenomenon called magnetic frustration, in which magnetic moments do not have clear choices of how to arrange themselves in simple arrangements, and the outcomes often are complex and intricate forms of magnetic order. In certain cases frustration causes magnetic moments to form a spiral around rows of atoms. The unexpected surprise is that these magnetic spirals induce ferroelectricity and provide the opportunity to switch the direction of the ferroelectric alignment in the material with a magnetic field. This effect is highly desirable for technology, but was thought to be too weak an effect to exist in Nature – a notion now known to be just wrong. New and strange magnets that have such unique magneto-electric effects are constantly being discovered. Indeed, distilling the key features of frustration into a chemical language could help to discover new materials with these novel properties. Once these materials are found, it will be critical for us to understand the novel and often complex magnetic order that produces their novel magneto-electric properties. Practical magneto-electric devices need spiral magnets that work at room temperature and which are cheap to make. Copper oxide based materials may be suitable candidates. The intense neutron beams of the ESS will be required to probe the magnetic structure and dynamics of ultra-thin magneto-electric films that will be used in such devices, which need to operate at the nanoscale of current computer circuits.

These new multifunctional materials prove to be increasingly complex in their crystal and magnetic structure, and corresponding behaviour. Polarised neutron studies are absolutely critical in determining how the magnetic moments align in these materials, and how they are affected by external electric and magnetic fields. The bright and polarised neutron beams of the ESS will allow us to peer deeply into these emerging materials.

Self-organising surfactants. Adding a detergent to a mixture of oil and water causes the oil to dissolve. This is what happens when we wash dishes. Washing-up liquids contain surfactants – long chain molecules with hydrophilic heads and hydrophobic tails. These materials are produced and used in huge quantities (about

9 megatonnes per year) in everyday life, industrial processes and in Nature. They are used in cleaning products as well as in foods, cosmetics and pharmaceutical products. Surfactants are also the main components of cell membranes.

A key property of surfactants is that they self-organise into nano-sized aggregates with a large range of structures, shapes and sizes. They can also form hierarchical structures over a broad range of length scales. The result is that they can form highly complex, functional fluids of great commercial interest, especially when mixed with other materials. Furthermore, with the advent of nanotechnology, it becomes very interesting to study the self-assembly process with a view to creating artificial nano-structures.

Despite their importance, such processes are still poorly understood. While neutron scattering has already proven to be a powerful tool in investigating surfactants, the ESS will offer the opportunity to probe behaviour at previously unexplored length and time scales. This will allow us to learn much more about surfactant aggregates and their self-assembly. It will lead to a better understanding of natural processes (and why they go wrong in diseases), as well as methods to optimise industrial procedures and produce advanced, more efficient and environmentally friendly materials. Furthermore, by mimicking their self-assembling behaviour, we might produce nano-structured materials or nano-machines.

Neutrons and heritage. Neutrons offer the opportunity to look at fossils, ancient artefacts and works of art, probing their texture and inner structures non-invasively. Intense and highly focused neutron beams offer exquisite spatial resolution within minutes, if not seconds, revealing crucial information about an item's origin. Museum experts will be able to decipher the methods used by artists and craftsmen, by detecting details of microstructure and composition of artefacts. Pigments in paints and glasses will be scrutinised and monitored, and forgeries will be easier to detect. High neutron sensitivity and bright beams also provide support for conservation programmes for buildings and sculptures by allowing the study of porosity, corrosion or erosion, and even the migration of water in materials. Neutron imaging of geological fossils will routinely reveal their interiors. The superb contrast obtained with neutrons will provide archaeologists and palaeontologists with extraordinary images of the inner structure of stones, fossils and bones, with a spatial resolution of a micron. Neutron techniques will become better known and amenable to a wide community of users who will see with neutron eyes.

The power of curiosity-driven research. Curiosity is one of the main driving forces behind human progress. Discoveries that seemed to be entirely disconnected from everyday life when first made often lead to the most remarkable technical advances at a later stage. The discovery of the electron in the 1890s was then thought to be "of no use to anyone", when the British physicist J.J. Thomson investigated the mysterious rays emanating from a cathode in a discharge tube. Later, in 1911, the Dutch physicist Heike Kamerlingh Onnes, wanting to find out what happened to the electrical conductivity of metals at temperatures close to -273 C (absolute zero), discovered that mercury lost all electrical resistance and became superconducting. This exotic electronic phenomenon, found in such extreme conditions, was not of obvious use and was explained by quantum physics only years later. The magnetic resonance imaging (MRI) scanners routinely used in hospital diagnosis now depend on superconducting technology. Today, our society depends crucially on our understanding of the behaviour of electrons – for example, in chemicals such as drugs, and in computer chips and other electronic devices. But it is still difficult to predict just how curiosity-driven discoveries will turn into spectacular applications.

Investigating new states of matter. Physicists continue to explore complex electronic behaviour and the underlying quantum physics, sometimes under extreme conditions. Neutron scattering is ideal for investigating exotic electronic materials because both neutrons and electrons have a magnetic spin. A beam of neutrons can magnetically interact with electrons in a sample to give a scattering pattern that provides information about their spins. Fortunately, the neutron has no charge, otherwise the charge interaction would completely hide the magnetic information.

One notable success for neutron scattering experiments involves superconducting materials that allow lossfree electrical transmission. Unfortunately for their technical application, all known superconducting materials require significant cooling. Although it is understood why so-called "conventional" superconductors become superconducting, the origin of superconductivity in "unconventional" superconductors – which exhibit the highest (and hence the most interesting) superconducting transition temperatures – is still unknown. Neutron scattering experiments show that magnetism and superconductivity are interwoven in all of the several classes of unconventional superconductors that are currently known. Our understanding of superconductivity is constantly challenged and advanced by every unpredicted discovery of a new material. The unique potential of neutron spectroscopy reveals the role that magnetism plays in these exciting materials. Understanding the microscopic details better and eventually learning to create superconducting materials close to ambient temperatures would have a tremendous impact on society.

The description of electrons in metals as free particles is arguably one of the most successful concepts in solid state physics. Nonetheless, the underlying concept of a "Fermi liquid" not only fails when understanding superconductors, but also when applied to many other technologically interesting materials, including those in which electrons interact strongly with each other to form a "non-Fermi liquid". The properties of these materials depend dramatically on the exact alloy composition, on subtle competing electronic interactions and on quantum effects. Neutrons are a unique tool to study these new states of matter, due to their sensitivity to magnetism, their power to reveal structural details and the capability to identify the relevant energy scales.

The benefits of frustration. Many types of exotic magnetic structures are being studied, in which the magnetic moments can arrange themselves in two or more ways in their lowest energy state. This results in so-called frustration, when the magnetic moments are disordered in a similar way to the disordered atoms in a glass. These materials are called spin glasses. They are of wider interest because the theory describing them can be applied to other analogous, but completely different, situations.

A good example is that spin glasses can mimic how neurones in the brain transmit and store information – in other words, they mimic memory. The complex tasks carried out by neurones and synapses can be described by computer models known as neural networks. These have found an enormous amount of success not only in academic research but also in spectacular real-world applications where artificial intelligence is needed, such as flying unmanned aircraft or recognising credit card fraud. It turns out that they are also an excellent tool for exploring the frontiers of knowledge of the physical world – interactions between electrons in a spin glass are similar to those between neurones in a neural net. Using the ideas of spin glasses derived from looking at magnetic materials, neural networks can be constructed to correct transmitted electronic signals that have been corrupted by background noise. Neutrons can provide detailed information on how the electron spins are arranged in spin glasses, and how they move in time, and so test improved theoretical models that lead to progress in neural networks and our general understanding of materials. Such experiments are currently intensity limited. With the powerful beams produced by the ESS, detailed comparison between experiments and theories will be pushed to unprecedented precision.

Understanding the universe. As well as acting as a probe of materials, the neutron can also be used to find out more about the fundamental forces governing the universe. The neutron has no charge, and in a universe with perfectly symmetrical forces it would also have no electric dipole moment (EDM). However, we know that the universe now contains much more matter than antimatter, which could have happened only if this symmetry were partially broken during primal events just after the Big Bang. Current theories describing how the fundamental particles and forces came into existence will need radical revision, depending on the value of the EDM, and so researchers are trying to measure the neutron EDM incredibly accurately, using neutrons at very low energies. Another exciting group of experiments investigate the nature of gravity. An outstanding challenge is to reconcile quantum theory, used to describe particles like the neutron, with Einstein's theory of gravity. By studying the reflection of very slowly moving ultra-cold neutrons off an extremely flat mirror, it can be shown that they reside in discrete layers above the surface and "bounce" in discrete steps, confirming that their gravitational energy has a fixed set of values: the energy is quantised. Ingenious neutron experiments are being planned to investigate gravity further.

2.1.4 The ESS challenge

The diverse examples described above illustrate that neutron scattering is not a single technique limited to solving a single problem. Rather, it encompasses an arsenal of modern methodologies with the potential to further our understanding in a broad range of scientific quests. The suite of 22 instruments currently being developed will best exploit the high intensity, long pulse ESS neutron source. This quest entails novel solutions and explorations of new technology. Each research area requires different instrumentation. Each instrument will have specific characteristics and layout, and these specifications will determine the capabilities of that instrument, defining to an extent the science that can be pursued there. Thus, the current development of a balanced instrumentation suite is of utmost importance to the scientific success of the ESS. For that reason, the international neutron science community – both instrument developers and users – is involved in the discussion of which kinds of instruments need to be included, and which requirements must be met. This is therefore a comprehensive process, including scientific discussions of promising new research directions, consolidation of currently strong fields within neutron science, and technical development of state-of-the-art neutron scattering instrumentation.

Humanity continues to breach the limits of what is technologically possible, advancing the frontier of technical solutions and expanding the level of understanding of the natural materials surrounding us. Front-line research

infrastructure and leading edge research technology is at the heart of progress, as we proceed into the future. It is not clear whether the next big breakthrough will be in green energy, novel materials, medicine, or in our fundamental understanding of matter – but the challenge is clear: to develop the ESS in a way that will accommodate the science of tomorrow.

2.2 Instrument suite

2.2.1 Instrument selection

A total of 22 instruments will be built to serve the neutron user community, with the initial 7 instruments coming online with the first neutrons in 2019, and the full suite available for the user programme in 2025. A strawman 22-instrument suite is listed in Table 4, with the corresponding layout shown in Figure 5. Experience at existing neutron centres indicates a 5-year construction schedule for an instrument once the conceptual design has been agreed on. Based on this estimate, we envisage giving the go-ahead for construction for the first three instruments in 2013. From then on until 2020, an average of 2.5 instruments will move into construction every year.

The method for the selection of instruments is an open process in which the scientific community is engaged and assumes ownership of the choices made. Instrument concepts are proposed by scientists in partner countries and are then incorporated into the ESS programme after endorsement by the Scientific Advisory Committee (SAC). When the conceptual design of an instrument reaches a sufficient level of maturity, a proposal to build the instrument can be submitted, which will then be evaluated in a peer-review process, with well-defined scientific and technical evaluation criteria. The process will repeat every year until the full instrument suite of 22 instruments has been selected.

The instrument suite presented here follows the instrument recommendations made by the ESS SAC in 2010 and 2011. It focuses on the natural strengths of the long pulse concept in order to maximise scientific output and considerable effort has gone into developing novel concepts for optimising long pulse performance. It cannot represent the precise instrument suite that will actually be built, as the process of choosing instruments for construction has only just begun. Instead, the presentation of the instrument suite is intended to give an overview of the current state of the instrument design effort, and shows the expected performance and possible scientific impact of the instrument suite.

The instrument design concepts outlined in this chapter are the result of an ongoing work effort, distributed among many laboratories and universities throughout Europe. The majority of the design effort is organised into Work Packages, using manpower at participating laboratories and universities, provided as national in-kind contributions to the ESS project. The establishment of the science drivers for the various instrument types is also an ongoing process, using input both from appointed advisory panels and open consultations with the user communities. The instrument designs are driven by the science drivers for the individual instruments. They necessarily reflect the scientific perspectives as they present themselves at the time of writing.

The description of the strawman instrument suite is arranged into instrument classes, depending both on the length and energy scales to be probed and the type of sample. Ten different instrument classes have been defined:

- 1. Reflectometry,
- 2. Small-angle neutron scattering,
- 3. Powder diffraction,
- 4. Single crystal / magnetism diffraction,
- 5. Macromolecular diffraction,
- 6. Engineering diffraction,
- 7. Imaging,
- 8. Spectroscopy for fast dynamics,
- 9. Spectroscopy for slow dynamics, and
- 10. Hybrid instruments.

2.2.2 Reflectometry

Science drivers

The advanced thin film materials of the future will be increasingly complex and thus there is a strong continued need for high-performance neutron reflectometers to elucidate their structure. Given the strong European base of reflectometry, there is also a need to be ambitious and differentiate the ESS reflectometry

Sector	Port	Angle [deg]	Instrument name	Length [m]
EAST	1	-17.5	Wide angle spin echo	25+3
	2	-22.5	_	
	3	-27.5	Extreme conditions spectrometer	30 + 3 + 2
	4	-32.5	Test beamline	35 + 2
	5	-37.5	Extreme conditions diffractometer	25 + 3 + 2
	6	-42.5	_	
	7	-47.5	_	
	8	-52.5	_	
	9	-57.5	_	
	10	-62.5	_	
	11	-67.5	_	
	12	-72.5	_	
SOUTH	1	-82.5	_	
	2	-87.5	_	
	3	-92.5	Vertical sample reflectometer	56
	4	-97.5	Multi-purpose imaging	56
	5	-102.5	Fundamental Physics beamline	81
	6	-107.5	SPEED engineering diffractometer	81
	7	-112.5	Hybrid diffractometer with SANS & Imaging	81
	8	-117.5	Bispectral chopper spectrometer	81
	9	-122.5	General Purpose powder diffractometer	81
	10	-127.5	_	
	11	-132.5	_	
	12	-137.5	_	
NORTH	1	17.5	Small sample SANS	14 + 2
	2	22.5	High resolution spin echo	22 + 3
	3	27.5	Conventional SANS	20 + 12
	4	32.5	Horizontal sample reflectometer	30 + 5
	5	37.5	Grazing incidence SANS	20 + 12
	6	42.5	_	
	7	47.5	_	
	8	52.5	_	
	9	57.5	_	
	10	62.5	_	
	11	67.5	-	
	12	72.5	_	
WEST	1	82.5	Narrow Bandwidth Powder diffractometer	156
	2	87.5	Crystal analyser spectrometer	156
	3	92.5	Magnetism diffractometer	156
	4	97.5	Macromolecular diffractometer	156
	5	102.5	Cold chopper spectrometer	156
	6	107.5	-	
	7	112.5	-	
	8	117.5	_	
	9	122.5	-	
	10	127.5	-	
	11	132.5	Backscattering spectrometer	300
	12	137.5	Thermal chopper spectrometer	300

Table 4: Preliminary instrument angles, names and lengths, as shown in Figure 5. Where a single length is given, the number refers to the distance from the moderator surface to the sample on the instrument. When the length is expressed as a two-term sum, the first term is the moderator-sample distance and the second term is the sample-detector distance. For the three-term sums, the first term is the distance from the moderator to a crystal monochromator, deflecting the beam to the side. The second term is the monochromator-sample distance, and the third is the sample-detector distance.



Figure 5: Preliminary neutron beamline and instrument layout, for the instruments listed in Table 4.

suite from existing instruments. The chemical and structural complexity of the systems studied by reflectometry has significantly increased during the last 10 years and many experiments now involve both specular and offspecular measurements, as well as grazing incidence small angle scattering and diffraction. Complementary and *in situ* techniques (such as X-ray reflectometry, ellipsometry, Brewster angle microscopy and infrared/Raman spectroscopy) are also often needed to elucidate complex structures and processes that are difficult to reproduce exactly. For both biological and magnetic materials, the sample sizes required by neutron reflectometry (NR) today are so large that rare proteins and advanced device structures cannot yet be studied. In both cases the experimentally accessible Q range is also flux limited. Thus, there is a clear and urgent need to use the high flux of the ESS to reduce the beam footprint and thus to minimise the required sample size.

Minimising the beam size will also enable studies of real interfaces that are not perfect: rough and curved interfaces are common in functional and natural materials (industrial coatings, ball bearings, bone, skin et cetera.), whereas other inhomogeneous or structured surfaces could thus be scanned for local features. The future materials studied by reflectometry will increasingly include both inorganic/magnetic and soft/biological components, and the traditional soft and hard condensed matter fields are converging in that polarised neutron beams, smaller samples and lateral structure determination will be universal requirements for reflectometry at the ESS [7].

Challenges in soft matter and biology. The systems of interest span air-liquid, liquid-liquid and solidliquid interfaces, biological and non-biological systems of amphiphilic and self-organising character. In all of these NR offers a unique possibility to probe the nanoscale structure and chemical composition. The high flux of the ESS will allow the study of smaller samples and faster kinetics in all the above areas, but of particular interest are the:

- Biological and bioactive samples of medical relevance, which need large high throughput screening of activity/structures, and where the available sample amounts are in the μ g range or less.
- Liquid-liquid interfaces (for example oil-water), which are of significant technological interest, but have been difficult to study with NR due to the drastic beam attenuation by the liquids. The ESS flux will offer a significant reduction in the experimental path length needed to obtain a good signal-to-attenuation ratio at grazing incidence when the beam traverses the full length of the liquid phase.
- Magnetised reference layers, which offer additional contrasts and sensitivity to fragile samples in which other forms of contrast variation cannot be used. Thus, a polarised beam with optional polarisation analysis should also be available on a reflectometer dedicated to biological and soft matter.

The length scales of interest in soft and biological systems span 1 Å-1000 Å, and require an instrument with variable resolution. The ability to approach the interface below as well as above the sample horizon is important for many buried interfaces, as well as for complementary *in situ* measurements or sample environments (for example shear cells or microscopes).

Due to strong development of high flux time-of-flight NR instruments at both ILL and ISIS in recent years, the focus in soft and biological condensed systems has moved to following increasingly fast time-dependent processes at interfaces. Today, large samples (30 mm \times 100 mm) are used to reach 1 s time resolution on world-leading instruments, such as FIGARO and D17 at the ILL. At the ESS it should be possible to reach sub-second time resolution on samples that are of comparable size to today. Hence, in order to make use of the highest possible flux gain for samples which can be obtained in large sizes, the maximum illuminated sample area should not be overly restricted. As the timescales decrease, the number of measurements and samples will also increase significantly at the ESS, which means that automated, efficient and reproducible ways of handling both samples and the data are needed.

Challenges in hard condensed matter and magnetism. Polarised neutron reflectometry (PNR) remains the only technique that can probe the internal magnetic structure of thin films, which do not necessarily have the same properties as their bulk counterparts due to surface effects, such as strain and oxygen deficiency. Although the total film thickness can be up to 2000 Å, such interfacial effects are only resolved at high Q as the unit cell dimensions are of the order of 5 Å. For the same reasons, the resolution requirements are as broad as for soft condensed matter, although the emphasis is on medium-high resolution. The main challenge in studying magnetic films today is that the samples are typically very small ($\leq 5 \text{ mm}^2$). The ESS flux should enable higher resolution studies on small samples, since there is also a real need to focus on even smaller samples as many functional devices are only grown on areas of 100 μ m × 100 μ m or less. There is also increasing interest in lateral information on 2D structured samples (for example magnetic nanodots, 2D superlattices, spin ice), and measuring canting of magnetic structures by diffraction measurements (since very few polarised diffractometers now exist). For these purposes, there is need to optimise the required collimation on small samples, which could also be used to obtain local information. While there is less need for dynamic measurements on short timescales compared to soft matter, functional studies of magnetic films involve scanning temperatures and field strengths, making efficient data collection up to high Q on relatively short timescales important. High efficiency in polarisation and polarisation analysis are essential to be able to detect increasingly small magnetisation, and emphasis will be placed on optimising this for time-of-flight measurements at the ESS.

Horizontal sample reflectometers

A horizontal sample reflectometer is necessary in order to study free liquid interfaces. Although many users ignore polarisation analysis today, in 10 years time it may be of standard use due to the increasing hybrid nature of advanced materials. Thus the instrument should be equipped with polarisation and polarisation analysis, and should be of interest to both hard and soft condensed matter scientists. Possibilities to fulfil the collimation and resolution requirements for GISANS should be investigated. The instrument should cover length scales between 10 Å-1000 Å and have variable resolution from $3\% \leq \Delta \lambda/\lambda \leq 10\%$. The beam should allow larger sample sizes of up to 40 mm \times 80 mm to be illuminated, with the possibility to focus efficiently on smaller samples (10 mm \times 10 mm). The length of the instrument should be optimised for the best compromise between the dynamic wavelength range and resolution so that kinetic studies on the seconds-to-minutes timescale can use a dynamic bandwidth (2-10 Å) sufficient for structure determination in 50 Å thin films. The minimum accessible Q range 0.005 < Q < 0.5 Å⁻¹ should be accessible from either above or below the sample horizon in 2-3 angles of incidence without tilting the sample. It is foreseen that the instrument will need to be equipped with a set of pulse-shaping choppers to obtain higher resolution for the study of static structures. For specular measurements, the beam should be strongly focusing in the horizontal direction in order to maximise the flux on the sample. The vertical optics need to move the sample out of direct line-of-sight of the source and also eliminate the longest wavelengths using a frame overlap mirror or chopper. For free liquid samples, the neutron guide will be inclined at a small angle. Extra attention will be paid to reducing background, which is one of the main limiting factors in the accessible Q range. Different strategies for optimising this instrument for off-specular reflectivity from small, weakly scattering samples will also be considered.

High flux horizontal instrument for small samples. This is a general purpose horizontal instrument, capable of catering for both the soft and hard matter communities [8]. The primary aim of this concept is to use the flux gain at the ESS to reduce the sample size for studies of free liquid interfaces on biological and soft matter samples, while including a polarised beam for magnetic contrast variation studies, and optional polarisation analysis. The instrument will however not be fully optimised for ultra-small samples requiring extreme collimation to $< 1 \text{ cm}^2$. The instrument should have a relatively low intrinsic resolution, which may be improved by the use of Wavelength Frame Multiplication (WFM). Using the full pulse width implies a relatively short instrument of the order of 25–35 m, which is primarily limited by the lowest acceptable neutron wavelength resolution, which in turn is limited by the lowest wavelength used. Figure 6, which shows the relative resolution $\Delta t/t$ as a function of the wavelength for different instrument lengths, indicates that the instrument should not be longer than 30 m from source to detector in order to have a usable wavelength band from 2–10 Å, giving a relative resolution of 19% for 2 Å.

Such low resolution values are used on existing instruments (for example D17 at ILL) when the required Q resolution allows this. To improve the limiting value of the resolution, it is possible to move the wavelength band to higher wavelengths, which however limits the instantaneous Q range. Using 2–10 Å it is possible to cover the minimum desired Q range for most applications (0.01 < Q < 0.4 Å⁻¹) with three angles of incidence. Ideally the instrument would have a freely variable angle of incidence up to at least ±4 degrees, which would be achievable using an inclined guide and a single m = 7 supermirror. However, the use of two m = 6 or m = 5 mirrors is also being considered. The mirrors should be followed by a final collimation guide to eliminate off-specular background. The beam sizes needed for reflectometry do not usually exceed 5 mm vertically and 30 mm horizontally even on very large samples, and the beam size extracted from the source only needs to be of the order of 10 mm × 100 mm. Different beam optics will be considered, such as elliptical and/or parabolic guides or a conventional straight-guide, two-slit arrangement. For GISANS, another collimation guide is required to allow horizontal focusing onto the detector without increasing the beam width at the sample beyond 30 mm. The sample-detector distance should be variable from 1 m to the distance required to reach sufficient Q_y resolution and range in GISANS (typically 12–15 m with today's detector resolution). Ideally the instrument will have a modular structure to allow the placement of an Neutron Spin Echo (NSE) add-on (for example SERGIS).

Multi-beam reflectometer with extended simultaneous Q range [9]. One of the main challenges for reflectometry at the ESS will be to overcome the intrinsic limitation in simultaneously accessible Q range,



Resolution and bandwidth

Figure 6: Relative time resolution as function of wavelength and instrument length.

which should be as broad as possible for fast kinetic studies that allow structure determination. Measuring several angles of incidence simultaneously could solve this problem, but in order not to increase the background proportionally, it is necessary to decouple the angles from each other in time, at the single pulse level. Such an instrument could be realised using 3 fixed angles (up or down, or both) to cover a Q range of 0.01-0.4 Å⁻¹ simultaneously. Since the sample reflectivity falls as Q^{-4} , it will be necessary to measure an increasing number of pulses with increasing angle of incidence to reach the required statistics. This can achieved by a fast beam selection chopper/slit/shutter which opens the beam to each angle for the desired number of pulses, for example 1, 2, 4 pulses into angles of, for example, 0.6° , 1.6° and 3.6° , which would give the measurement an effective time resolution of 0.5 s at the ESS frequency of 14 Hz. The instrument can in principle be polarised and the construction of a multi-guide system should not present significant challenges if the instrument is aimed at small sample studies, in which case each guide could only be $10 \text{ mm} \times 50 \text{ mm}$. The instrument would be one of a kind and would give access to an unchallenged simultaneous Q range, which would allow fast kinetic studies of structural changes not possible on even the broadest band reactor instruments. The possibilities of using WFM for variable resolution are being explored, as well as options for a modular set-up, allowing different collimation options for GISANS or a SERGIS add-on.

Long narrow-band instrument for high resolution studies without WFM [8]. Since a reflectometer has not been built at a long pulse source such as the ESS before, it is of interest to compare the performance of a short high-flux instrument using the full pulse width and WFM to that of a long instrument with higher resolution without WFM, in which case broader wavelength bands can still be used by skipping one or more pulses. Both WFM and pulse skipping lead to a reduction in the effective flux and it is necessary to determine which method is most suitable considering the scientific drivers for reflectometry. The long instrument will otherwise be similar in construction to the high flux horizontal instrument, but will have a length of up to 150 m. It may be that this design will be more relevant to an instrument aimed primarily at the hard condensed matter community with higher resolution requirements, and could also offer a significant reduction in environmental background.

Vertical sample reflectometers

Polarised vertical reflectometer [8]. A second reflectometer should be vertical (for better access to higher angles) and polarised and preferably also have the capability to perform polarised GISANS. The vertical reflectometer should address the need to focus on very small samples and to be built considering the use of high magnetic fields. However the instrument would also be well-suited to the study of liquid crystals, membrane diffraction and a range of studies at solid-liquid interfaces. This instrument should cover a wide Q range, and be able to probe length scales between 5 Å and 1000 Å with variable Q resolution. It must be equipped with

polarisation analysis from the beginning. The layout of the instrument remains to be defined, but it should be optimised for flux considering very small samples. The length and resolution of the instrument need to be optimised, keeping in mind that solid samples do not necessarily require very fast kinetics studies. The background should be optimised so that the reflectivities recorded will only be limited by the samples. The ability to probe larger samples and having some overlap with the science drivers of the horizontal instrument would be advantages. The key performance parameters of the vertical instrument are:

- Sample size: $\leq 5 \text{ mm} \times 5 \text{ mm}$ taking into account sample environments
- Wavelength resolution: up to $10\% \Delta \lambda / \lambda$, with options to improve to 5%, 3% or 1%.
- Minimum Q range: 0.005 < Q < 0.5 Å $^{-1}$ measurable in 3–4 angles of incidence
- Access to higher angles up to 120°
- Low background: reflectivities $\leq 10^{-9}$ measurable at air-solid interfaces

SELENE concept [10]. SELENE is a novel concept (illustrated in Figure 7) for focusing reflectometry using an angular divergence of up to $\sim 2^{\circ}$ to illuminate a sample with a continuous spread of angles simultaneously. The angle of incidence is resolved by an area detector and the method is also suited to time-of-flight measurements using a white beam. The advantage of SELENE is that a relatively broad Q range can be recorded simultaneously with only the desired neutrons delivered to the sample. Test experiments done up to date at PSI have shown that flux gains of the order of 10 and 100 can be achieved by using elliptical focusing in one and two directions respectively. The disadvantage of the wide divergence concept is that it cannot be applied to samples with any form of off-specular or diffuse scattering. However, the system of two semi-elliptical reflectors is flexible and can be used in several other modes including a low divergence mode equivalent to a normal two slit instrument (Figure 7, bottom). The system may also lend itself to an equivalent of a multi-beam instrument by selecting several angles from the full divergence with a fast chopper or slit. The concept is expected to work better in a vertical geometry than a horizontal geometry, where the effects of gravity are less complicated. The wide-divergence mode is not applicable to liquid samples with strong incoherent/inelastic scattering, as there is no method to subtract the background, but the low-divergence mode still offers the advantage of a convergent rather than a conventional quasi-parallel beam. A horizontal SELENE-type instrument for liquid interfaces is therefore also being considered. The effects and possible elimination of off-specular background from the focusing supermirror need to be investigated. Test experiments using one semi-elliptical reflector on AMOR at PSI indicate that the method could be of significant interest for fast scanning broad parameter ranges, for example field strengths or temperatures at relatively low Q values, with the main application being ultra-small samples (for example devices) in the mm to sub-mm size range. A full test version of the concept will be realised at PSI on the test beamline BOA in 2012.

Spin-Echo-Resolved Grazing-Incidence Scattering (SERGIS) add-on [8]. Neutron spin echo encoding of the reflected neutrons can be used to decode the off-specularly scattered neutrons for better resolution and access to larger length scales than in conventional grazing-incidence scattering without the need for tight beam collimation. There may also be opportunities to use it as a means to eliminate some of the incoherent sample background. The addition of a modular NSE capability will be investigated in conjunction with both types of reflectometers for the ESS, with particular attention being paid to the requirements set on other measurement capabilities of the instrument. Since the NSE signal is relatively weak, it is anticipated that the method is not suitable for ultra-small or very weakly scattering samples. Similarly to GISANS, the method also relies on continuing theoretical developments for accurate modelling and analysis of data.

2.2.3 Small Angle Neutron Scattering (SANS)

Science drivers

Small angle neutron scattering has a broad, established user base. The science drivers presented here represent the view at the time of writing and will evolve further in 2012. The "big three" constituencies for SANS are structural biology, soft condensed matter and hard condensed matter. The needs of these constituencies often overlap and play to the strengths of the ESS source.



Figure 7: The SELENE concept. Top: The high-intensity wide-divergence mode, suitable for fast scanning of external parameters, but less so in the presence of off-specular scattering from the sample. Bottom: The low-divergence near-conventional mode, with which off-specular measurements can be made. In this mode the beam is still converging on the sample, helping to limit unwanted scattering from, for example, sample environments.

Structural biology. In the case of biological samples there are currently two main restrictions in the application of SANS. The first is that of sample size as often only small quantities of a protein can be expressed for analysis, particularly if deuteration is required. Traditionally SANS has required large (~ 1 ml) sample sizes leading to very low concentrations of sample in solution (as a result of small amounts of protein available) and hence poor signal-to-noise ratio. The second restriction is that of the incoherent solvent background. In many cases, the behaviour of the biological molecule is different in heavy and light water. Thus, it is often preferable to measure in light water, which leads to a large background signal limiting the size range that can be effectively studied.

The key improvements that can be achieved are thus related to using the flux to allow smaller sample sizes, allowing higher concentrations or at least matching the amount of material being produced for analysis by other methods. Additionally, high flux allows screening of large numbers of very small samples in a high throughput manner similar to synchrotron SAXS experiments, which would allow many samples not accessible in large enough quantities today to be studied using SANS, particularly those of biomedical and/or pharmaceutical relevance. Suppression of the incoherent background could significantly improve the applicability of SANS to biological molecules in the 5-20 nm size range and also potentially open up the accessibility of the technique since an improved signal-to-noise ratio may allow more experiments to be performed without expensive deuteration of the protein. Added to these benefits is the fact that Time-Of-Flight-SANS (TOF-SANS) is ideally suited to measuring relatively broad Q ranges simultaneously, for monitoring kinetics and dynamics of (for example) protein or ligand binding, conformational changes, aggregation and exchange processes.

Soft condensed matter. In soft condensed matter the sample sizes are not as limited by the availability or cost of the materials as they are in biological samples, and the flux gain should allow the study of kinetic processes in the millisecond range on samples of typical current size. Applications range from stopped-flow mixing to rheological processes. Many materials (for example gels, ceramics, and geological materials) have structure at a broad range of length scales of interest from 5 Å level up to several microns, and there is an increasing need for instrumentation that can reach both very low and relatively high Q values, from 10^{-5} Å⁻¹ to 0.5 Å⁻¹. These "hierarchical systems" present a significant challenge to existing instrumentation, often with multiple instruments and non-neutron techniques involved. The ESS has the potential to enable instrumentation with a very broad Q range, expanding the study of these types of system. Additionally, many soft matter systems have structure of interest from 5 Å up to hundreds of nanometres and there is a need to be able to investigate kinetic processes in such systems. TOF-SANS has an advantage here and very broad simultaneous Q ranges can be covered by the use of additional detectors.

Hard condensed matter. One of the main challenges for magnetic materials is also the sample size, which can be of the order of $2 \text{ mm} \times 2 \text{ mm}$. Micro-focused neutron beams would be of great potential interest for detecting local versus global structures, and scanning lateral inhomogeneities. The key needs for this constituency are high flux and excellent spatial resolution. They will be examined further in 2012.

Surface structures – Grazing Incidence SANS (GISANS). Although the previous discussion has so far focused on bulk samples, nonetheless all three SANS constituencies are also interested in surface structures. The user base for such experiments spans the existing user communities of both SANS and reflectometry. While the lateral topology of surfaces, both wet and dry, can be imaged with AFM and SEM, only neutron scattering can give both chemical and depth information *in situ* without damaging the samples. Neutrons can access length scales below the resolution limit of optical techniques and GISANS also measures the nanoscopic structure with statistical meaning, that is, it measures the object geometry and size distribution as well as the spatial correlations.

The main challenges with GISANS are the need to extend the high Q limit, and data modelling, which need to go hand-in-hand with instrument development. High flux time-of-flight GISANS offers possibilities to extend the measurable dynamic Q range, and to probe the structure as a function of penetration depth of the different wavelengths simultaneously. Developing GISANS on horizontal sample surfaces would open up a whole new scientific field on free liquid interfaces, for which there currently exists only one instrument – REFSANS at FRM-II. Today the counting times are typically relatively long (~60 s), but the high flux at the ESS should, for example, allow the study of the kinetics of morphological changes, phase transitions and nucleation of domains.

Small sample SANS instruments

This is the first of the two types of SANS instrument proposed: a very short instrument for small samples and with a broad Q range in a single measurement optimised for small biological samples. The science case is very strong because it would allow small quantities of new biological samples to be investigated with SANS. Many samples are currently unavailable in the amounts required today. Such an instrument would also lead to a significant number of high impact publications.

Small sample SANS with a multiple detector array. Because of the long pulse and high intensity of the ESS a small sample SANS could be realised by a short instrument (for example 10+2+2 m sourcecollimation-sample-detector) which would make use of the whole 2.86 ms pulse and a dynamic wavelength band of approximately 3 - 20 Å. This instrument would cover a Q range from 10^{-3} Å⁻¹ to 1 Å⁻¹. Assuming a 2 mm × 2 mm pinhole beam and 10 times more neutrons than on a comparable instrument at the ILL, the intensity on the sample would only be 2.5 less than for a 10 mm × 10 mm sample at ILL. Such an instrument would be the best in the world, could be realised for moderate costs and would also pose few risks from completely new developments. However, since the detector is so close to the source (14 m) the background could be a problem. Direct lines-of-sight from the source need to be eliminated and solutions for optics need to be evaluated. The accessible Q range covers a suitably broad dynamic range. Due to the compact size of the instrument, the dimensions of the sample environment will be rather restricted. In addition the detector would need a high spatial resolution (~ 0.1 mm), a large area (1 m² for 1 Å⁻¹ at 2 m distance from the sample) and high count rate capability. The realisation of this concept therefore relies heavily on the development of high resolution detectors.

An alternative for a small sample instrument is a layout that has a detector at 24 m from the source and which simply collimates the beam with small apertures (Figure 8), with either pinhole or slit geometry. A high resolution mode with the position of the second detector at 27 m from the source is also included. To minimise the background in the first 6 m after the source (if possible) a system of mirrors and/or neutron guides would be installed – including a frame overlap chopper – to pre-define the beam such that it can be used in an optimised fashion in the following 8 m. Various options for collimation and focusing could be incorporated through the use of a flexible optics section. Since the optical section will flexible, fast changing optical elements to allow for optimal flux and resolution on each detector bank can be installed.



Figure 8: Schematic of a small sample focusing SANS.

Two detectors need to be installed, in order to reach the optimal dynamic range. For the maximum momentum transfer the first detector is positioned 1 m from the sample. The optimal solution is a movable setup that allows for positioning a detector at an angle (assuming for example boron converter tube detectors). A second detector positioned at 4 m allows for low Q detection. The dynamic range of the instrument operating with slit collimation (0.1 mm for lowest Q in the horizontal direction, 2 mm in the vertical) is 10^{-5} Å⁻¹ to 1 Å⁻¹, still achieving high intensities. A detailed simulation analysis of the best layout of the proposed components needs to be performed. A suitable area for the installation of large sample environments will be available, since the instrument is not limited in space. Furthermore, it will be relatively easy to implement additional options such as polarised neutrons and a spin analyser, which could be used to eliminate some of the incoherent background for soft matter and biological samples.
Compact BioSANS instrument with inelastic background suppression. The Compact BioSANS is a new instrument design that ideally combines optimum dimensions of the instrument for small sample volumes and an option to suppress the inelastic part of the incoherent sample scattering in order to increase the signal-to-noise ratio, and to extend the accessible Q range. A monochromatic pulsed beam is required, to suppress the incoherent inelastic scattering of the solvent. While this may not appear to be the best way to use a long pulse source, the advantages gained by the background suppression are significant and are very relevant: solvent scattering is the main limiting factor of the experimentally accessible Q range in dilute biological systems, severely restricting the structural resolution compared, for example, to small angle X-ray measurements. Thus, in order to take full advantage of neutron contrast variation experiments, using a monochromatic beam would be well justified in many cases. The improved structural resolution would significantly strengthen the standing of SANS in the biological sciences community.

The general instrument design could also be optimised for small sample volumes by scaling down the whole pinhole SANS geometry, maintaining the ratios of collimation length to neutron guide length, and sample cross section. The short design has the additional advantage of a broader Q range, as well as being capable of using the whole pulse length without frame overlap problems. The concept of inelastic background suppression can be incorporated in any general compact SANS instrument concept. The wavelength spread of the beam can be varied by either a supermirror acting as a wavelength band filter, or by a chopper. The suppression of the inelastic scattering of the sample is likely to be Q dependent. This is related to the diffusion coefficient of the sample and solvent molecules, as well as to the amount of multiple incoherently scattered neutrons (especially for highly protonated samples), and to the energy resolution or cut-off of the proposed setup for separating elastic and inelastic neutrons. A detailed simulation for this experimental setup in combination with corresponding test experiments will be performed.

The detector requirements of this concept are the same as for the general small sample SANS, discussed above. They rely on the development of high resolution, large area detectors with high count rate capabilities.

General SANS instrument

A longer instrument (for example 8+12+12 m) that will allow larger samples (10 mm \times 10 mm) and access to smaller Q with a better wavelength resolution is needed primarily for the general soft condensed matter studies in which the sample amounts are not as limited as in biological systems, and which exhibit structure on larger length scales up to several hundred nanometres. The reduction in wavelength range caused by the increased instrument length will be compensated by a larger or more flexible detector arrangement, coupled with more sophisticated beam optics. A fast collimation option moving at the pulse frequency is an option that could be used to optimise the flux and resolution on a flexible array of several detectors. Chopper configurations need evaluation and comparison with a long wavelength cut-off filter. Neutron optics for beam delivery, collimation and avoiding direct line-of-sight of the source need to be evaluated. This type of instrument can easily consider additional options such as:

- Polarisers using mirrors
- Polarisation analysis using polarised ³He
- Lenses
- focusing Mirrors
- Grazing incidence SANS
- Spin echo SANS
- Inelastic SANS, for example for eliminating inelastic background
- Wide angle detectors

Some consideration is also given to the possibility of including a general SANS component on one of the hybrid instruments including powder diffraction and/or neutron imaging techniques

Grazing-Incidence SANS instrument

Accurate alignment (to 0.02° or better) and illumination only of the surface of interest are absolutely essential in TOF-GISANS, so the instrumental requirements partly resemble those of a reflectometer. However, a GISANS instrument typically needs to be of a similar length to a conventional SANS instrument (~15 m) in order to obtain a sufficiently good collimation, Q range and resolution. It is not clear yet which instrument type would be better suited to a GISANS option, or whether a stand-alone dedicated GISANS instrument would be a technically superior solution with strong scientific drivers. All these options are being considered.

2.2.4 Powder diffraction

Science drivers

Powder diffraction is the cornerstone of materials characterisation and can be applied across a wide range of scientific disciplines. Knowledge of structure is essential in order to understand physical properties and to design new materials. Powder diffraction gives information about structure over a range of scales: long range structure in polycrystalline materials, local short range structure in highly disordered materials and, increasingly, intermediate structure through the use of total scattering measurements coupled with pair distribution function analysis. The complementarity of X-ray and electron diffraction with neutron powder diffraction is well known. The latter plays a key role despite being less commonly available.

The sensitivity of neutrons to light elements, such as H, Li, C and O, and the difference in scattering length between isotopes, such as H and D, finds uses in high impact technological areas such as ceramic materials, solid oxide fuel cells, lithium ion batteries, hydrogen storage materials, framework materials including zeolites, metalorganic frameworks and many others. The magnetic interaction between the neutron and the local magnetic moments within a sample mean that magnetic structure can be probed with applications across the whole range of hard and soft condensed matter physics from rare earth magnets and high T_c materials to molecular magnets, highly correlated electron systems and multi-property systems (ferro-electrics, magneto-electrics et cetera). The high penetration depth of the neutron makes it ideal for in situ experiments with specialised sample environment allowing measurements over a wide range of temperature, electric or magnetic fields, gas flow and varying pressure. Examples of applications include the study of phase transitions, geological samples under extreme conditions of pressure, very low temperature magnetic phenomena and, increasingly, in the field of chemistry to understand reaction pathways, kinetics and process. The combination of higher fluxes, event mode detection and large area detector coverage, coupled with optimised sample environments and the high penetration depth of neutrons, opens up possibilities in parametric studies and time resolved phenomena across fields of technological interest such as electrochemistry, catalysis, ceramic membranes used in SOFCs, hydrogen storage materials and charge/discharge in battery materials under working conditions as well as readily investigating smaller samples.

The powder diffraction science case broadly separates the instrument characteristics into two types – those that require high resolution and those that require high intensity. The resolution determines the limit to which the real space structural features of materials can be extracted and the intensity how fast such a measurement can be performed. The two properties are effectively inversely related and a high requirement for one results in a significant limitation on the other.

High intensity is the primary driver in two areas – weak scattering phenomena and process. The former would include experiments with small samples, weak signals, hydrogen containing materials and qualitative phase analysis whereas the latter includes time resolved experiments, reactive chemistry or catalysis and phase transitions. With high intensity the counting time is reduced and, with certain processes, can be limited by the time resolution of the neutron detection itself. Processes can be reversible, cyclic or irreversible and event mode neutron counting allows all of these types to be easily investigated without the requirement for stroboscopic acquisition sequences. Experiments in this category include chemical reactions, excitation phenomena (for example laser or ultrasound induced states and their decay processes) and rheology. Mapping the phase diagram for phase transitions requires many measurement points. Fast data collection allows finer resolution within the phase diagram and the possibility to investigate more materials in a given time period. Even in the simple case of mapping lattice constants as a function of temperature, subtle phase transitions can be easily missed.

Most new materials are only available in very small quantities and certain synthetic techniques only produce small samples (for example high pressure synthesis). Therefore, there is a real need for neutron diffraction instruments that are capable of measuring small sample sizes (< 10 mg and eventually μ g scale) similar to those required for analogous X-ray measurements. Other areas where small samples are the norm are thin film studies and extreme conditions (high pressure studies are limited to 10 mm³ or less). Hydrogen is probably the most important element in the universe and is of interest to communities from chemistry and physics across to the life sciences. It is a particular case in neutron scattering due to the large incoherent scattering cross section giving high background contribution. High intensity instruments allow the counting statistics to be high enough to extract accurate intensity information from these materials and also those with very weak scattering phenomena on reasonable timescales. The incoherent scattering can also be tackled by polarisation techniques and via energy discrimination, but each of these processes reduces the effective count rate of useful neutrons and so require very high intensity incident neutron beams.

High resolution is increasingly a requirement, as new materials tend to be more complex or differ from the structure of existing materials very subtly. A high resolution instrument allows peak splitting to be resolved yielding higher accuracy in the peak intensity required for a structural refinement. Great leaps forward have

been made in *ab initio* structure determination methods from powder data and the demand for resolution will be ever higher to tackle more complex structures. In many cases the properties are determined by the subtle deviation of the structure from some ideal or simple parent material. This is the case with catalysts based on zeolite materials, structurally and magnetically incommensurate materials, natural minerals, hybrid structures, nonlinear optics and others. High resolution is also required in cases of chemical phase separation and for subtle phase transitions – of high relevance to ferroic, electronic and magneto-resistive materials. Sample-related peak broadening can also be used on high resolution instruments to investigate strain, the presence of defects and crystallite size.

Clearly, the ideal powder instrument would have both high resolution and high intensity. However, this is very difficult to realise in a single instrument and so central facilities tend to build diffraction instrument suites of two or more instruments weighted toward one or other requirement. One of the advantages of a Long Pulse Spallation Source (LPSS) is that a single instrument is highly flexible, due to control over wavelength resolution, intensity and wavelength band via the chopper system and divergence from interchangeable or removable guide components. Additionally, with appropriate optimisation of detector geometry and pixel resolution, a powder instrument can also be used to perform pole figure measurements for texture analysis and single crystal crystallography and magnetism on unit cells up to those more suited to the dedicated macromolecular crystallography instrument (thermal cold guide wavelength versus flux crossover). A possible upgrade to a polarised neutron beam can also be built into any instrument concept, particularly if single crystal measurements are foreseen (WISH at ISIS for example).

It should also not be forgotten that sample environment is as important as the instrument in order to optimise the success rate and breadth of user experiments. Traditionally, central facilities have been weak in the provision of specialised sample environments outside of the temperature and magnetic field combination. This is changing with advances in high pressure equipment, gas flow, reactive chemistry cells and others, but neutron facilities need to learn from the X-ray world in this respect and engage the user community to provide as complete a suite of sample environment as possible to take full advantage of the capabilities of the proposed instruments. Background suppression from sample environment and other sources through adequate collimation and shielding is also a high priority.

Desired specifications for a powder diffractometer are:

- Average resolution $\Delta d/d < 3 \times 10^{-3}$ (< 6×10^{-4} for high resolution studies)
- Q range coverage $(0.1 < Q < ~\sim 50$ Å⁻¹, d spacing coverage $(0.1 < d < \sim 25$ Å)
- Flexible resolution and flux options (fully automatic)
- Focusing guide (interchangeable front end)
- Variable slits (automatic)
- Evacuated (or helium filled) beam path area
- Sub-second data collection (inherent for event mode acquisition systems)
- Fast detector read out (inherent for event mode acquisition systems)
- Large detector array (as large as allowed by sample environment geometry and focusing)
- High stability of detector
- Low background
- Large sample space for sample environment with good access
- Beam collimation pre-detector
- Smallest sample mass < 10 mg (eventually μg in high intensity mode)
- Typical sample volume $< 100 \text{ mm}^3$ (focusing requirements determine maximum sample size)
- Incident wavelength range $0.1 < \lambda < \sim 5$ Å (as wide as possible but determined by guide characteristics)
- Fully integrated data acquisition and sample environment control system

Three types of instrument can be conceived to address the requirements of the science drivers and are being investigated by the ESS partners:

- 1. Narrow wavelength band.
- 2. Wide wavelength band.
- 3. Monochromatic.

Each type has its strengths and weaknesses. For a thermal neutron powder instrument the wavelength resolution requirements are around 0.1% increasing to approximately 1% for a cold neutron instrument [11]. This requirement is inherently met for monochromator-based instruments but, for both the narrow and wide wavelength band cases, it is not possible to use the full pulse and a pulse shaping chopper is required. This tailors the pulse length to the required wavelength resolution, but at the price of a significantly reduced flux compared to the full pulse. At an LPSS, the natural instrument length is longer than that seen at either reactor or current SPSS facilities. This allows for a significant reduction in background contributions by bending out of line-of-sight of the source, which could justify construction of the instruments even if no other gain could be realised. Each of the broad classes for a thermal powder diffraction instrument is outlined in the following sections, with advantages and disadvantages listed. For comparison it should be noted that wavelength band instruments rely on the high peak brilliance of the long pulse source whereas monochromator based instrument require high average brilliance.

Narrow wavelength band instruments

This concept is being developed by the ESS partners to provide a baseline case and for instrument concept performance comparisons. The narrow wavelength band instrument concept is similar to that originally proposed for POWTEX at FRM-II (usable wavelength band of 1.4 Å) [12], and the POWGEN instrument at SNS (wavelength band approximately 1 Å). The instrument length is determined by the pulse length and the repetition rate and is around 150 m. The wavelength band is therefore approximately 1.8 Å ($\lambda_{max} - \lambda_{min}$). The wavelength resolution $\Delta\lambda/\lambda$ is continuously tuneable from < 0.001 to 0.042 (using $\lambda_{mean} = 1.8$ Å) using the pulse shaping chopper (better $\Delta\lambda/\lambda$ means lower flux on sample) and the band is tuneable over the whole spectrum provided by the moderator, assumed to be thermal, although a shift towards hotter neutrons would be a distinct advantage for total scattering experiments (access to $\lambda < 0.5$ Å). The instrument would operate primarily in angle dispersive mode due to the narrow wavelength band but this remains open to debate. Optimisation of the guide characteristics defines the maximum sample dimensions, the type of detector, its coverage and effective pixel size. There is a large parameter space to optimise before choosing the combination of guide, focusing, sample space, size and type of detector that best matches the science drivers. The figureof-merit to judge and compare different solutions must take into account more detailed information than the traditional figure-of-merit of detector area coverage multiplied by incident neutron flux, but it is clear that an instrument of this type would gain over a monochromatic instrument like D20 at the ILL and be more flexible than time-of-flight instruments such as POWGEN at SNS and GEM or POLARIS at ISIS.

The main advantage of the narrow wavelength band instrument is the flexibility inherent to the design. The wavelength resolution of the incident beam can be tuned with the pulse shaping chopper to suit the problem being investigated. The frame overlap chopper requirement and data reduction should also be simplified with a single wavelength band. There is also flexibility in the detector system. With appropriate guide focusing optics a 4π detector coverage could be used (like that proposed for the updated POWTEX concept [13]), a set of fixed angle cylindrical detectors (HIPPO at LANSCE), a banana-type detector of fixed radius (D19 at ILL or WOMBAT at ANSTO) on both sides of the sample position unlike at a reactor source, an exponential spiral (POWGEN at SNS), a typical SPSS detector arrangement (upgraded POLARIS at ISIS) or some combination approach. Access to sample position and optimisation for sample environment is possible with many of these detector geometries. Combination of optimised sample environment, event mode detection and the listed instrument advantages present a strong case for an instrument based on this concept and it would attract a diverse programme of science.

The main disadvantage is that the Q range covered is limited by the incident wavelength bandwidth at a fixed $\Delta d/d$ real space resolution in simple time-of-flight mode. The large scattering angle dependence of the resolution function means that useful $\Delta d/d$ values for crystallography ($< 5 \times 10^{-3}$) are only obtained at scattering angles greater than 120° in standard time-of-flight mode [12], hence the preference for angle dispersive or some combination detector approach. This can be overcome to a certain extent by arranging the detectors like those on POWGEN to minimise the effect of the variable resolution as a function of scattering angle but would still result in $\Delta d/d$ varying by more than an order of magnitude across the measured Q range. A narrower pulse could also be used but this would lead to lower flux and longer counting times. In order to cover the whole of Qspace with high resolution, several separate measurements would be required using different incident wavelength bands. In cases where a large Q range is required in real time (certain *in situ* experiments) this would be hard to realise without compromising on resolution requirements. The instrument length is very long compared with conventional spallation instruments and the cost of the guide and shielding would be a significant part of the instrument budget. The angle dispersive instrument setup also produces data that require significant effort in software development in order to analyse, as powder data would become multidimensional – see Figure 9.



Figure 9: A simulated powder diffraction pattern from POWTEX for angle dispersive data.

Wide wavelength band instruments (general purpose diffractometer)

Similar to the narrow wavelength band instruments, the concept uses Wavelength Frame Multiplication (WFM) [14, 15] to increase the width of the incident neutron wavelength band, as illustrated in Figure 10. As a result, the instruments are shorter and the detector arrangement becomes more like that seen at an SPSS – that is, as close to 4π as geometry allows – and the instrument layout would be very similar to the upgraded POLARIS at ISIS or its sister instrument GEM. An intermediate solution has been chosen for the updated POWTEX instrument at FRM-II based on a 2-band solution [13] with cylindrical detector geometry around 90° scattering angle and flat plate detectors at forward and back scattering positions and a similar instrument could be proposed for the ESS. The individual wavelength band remains 1.8 Å and the instrument length is proportional to the number of wavelength bands: n = 2 would be around 75 m long and n = 3 around 50 m. The wavelength resolution and bandwidth coverage would be tuneable.

The advantages are that a wide wavelength band is incident on the sample and so the Q range covered by a detector at a fixed scattering angle is also large. The guide system can be optimised to give almost spherical beam geometry at the sample with low horizontal and vertical divergence allowing large area detector coverage. There is also an advantage over conventional wideband SPSS instruments in that the pulse shaping chopper can tune wavelength resolution to flux incident on the sample for each individual wavelength band – relaxing the $\Delta\lambda/\lambda$ requirement as λ_{mean} increases. Using WFM reduces the length of the instrument considerably, with the obvious savings on guide and shielding. For instruments that have restricted geometry to just forward and back scattering, such as high field solenoids, a larger wavelength band is clearly the superior option.

The disadvantages include a complex chopper system to avoid band overlap within a frame and the fact that normalising data of this type has yet to be shown to be possible quantitatively. At constant $\Delta d/d$ there is a trade off in flux at sample for bandwidth. Simulation shows the trade off is close to inversely proportional – that is doubling the bandwidth gives half the flux per wavelength band at the sample position under constant resolution requirements and so no overall gain [16]. The flexibility to tune to a particular Q range is also reduced with this type of instrument. Very large area detector coverage also requires complex collimation and limits access to the sample position for demanding experiments. The preferred sample geometry is spherical and the maximum sample size is dependent on the guide focusing. It is also not possible to use a 4π detector array with restricted geometry sample environments in and out of the horizontal scattering plane or those that have large dead zones due to support structures (for example pressure cells). The gain over current short pulse source



Figure 10: Left: WFM showing multiple bands (n = 3 in this case) taken from a single initial pulse. Right: A single band instrument.

instruments is hard to judge and it is clear that a large part of the science case for an instrument of this type relies on very short wavelength neutrons, for which the long pulse concept offers no particular advantages.

Crystal monochromator instruments

This concept makes use of the fact that the time averaged flux of the ESS will be comparable to that of the ILL. The time structure of the pulse would be used for higher order discrimination and the instrument would be a conventional focusing monochromator instrument with flexible take-off angle geometry like D20 at ILL and WOMBAT at ANSTO. The science drivers for an instrument of this type are clear. The incident guide can be focused onto the monochromator to give a much higher flux than current generation instruments and be combined with an optimised 2-dimensional banana type area detector and event mode counting electronics. The possibility of horizontal focusing with respect to increase in flux versus loss in resolution at the detector (from divergence) and the limits this would impose on usable sample size need to be investigated.

The main advantages of an instrument of this type are the access to the sample position for complex user equipment. From a technical standpoint it is relatively easy to construct, the background can be significantly reduced with respect to a reactor instrument by lengthening the guide and bending out of line-of-sight as the cut-off in usable incident neutron wavelength is around 1 Å, but the instrument would remain short (< 50 m). Optimisation of the instrument would yield significant gains over D20 but through guide, optics and detector improvements rather than from source gains. The weaknesses are that the time structure of the pulsed source is not fully used, focusing monochromators limit detector geometry and size (the detector is a section of a hemisphere or a cylinder), the count rate on the detector would be very high during the pulse and zero otherwise (saturation of electronics, long term stability) and all of the optimisation could be performed at a reactor source, resulting in only a modest gain for the ESS instrument.

A further development of the crystal monochromator type instrument is the composite monochromator diffractometer. Here, several individual monochromators would focus the beam onto the sample, with wavelengths ranging from 1 Å to 2.5 Å. The arrival of each wavelength at the detector would then be separated using the detector time-of-flight capability, giving several full diffraction patterns per pulse. This requires monochromators that have high reflectivity and also high transmission, as they would be arranged in series with respect to the incident neutron beam exiting the guide to give a spread of incident monochromatic wavelengths (for example 1.0, 1.3, 1.6, 1.9, 2.2 and 2.5 Å). Feasibility studies are underway through in-house development and this instrument type represents a radically different approach. Access to a hot source would increase the potential impact of an instrument of this type.

2.2.5 Single crystal/magnetism diffraction

Instrument Concepts. The following list of preliminary requirements will be developed later:

- Many of the concepts for the protein crystallography instrument and powder instruments are relevant to this instrument class.
- A single crystal diffraction instrument equivalent to D19 at ILL, TOPAZ at SNS or SXD at ISIS is possible.

- Single crystal diffractometer for small molecules (similar to D9 at the ILL) would require hot neutrons and is not well suited to an LPSS.
- Single crystal diffractometer for magnetisation densities (similar to D3 at the ILL) requires hot neutrons and is not well suited to an LPSS.
- Single crystal diffractometer specifically for magnetism employing polarised neutrons and XYZ polarisation analysis using either ³He filters or supermirror analysers is well suited to LPSS. This instrument would outperform D7 at ILL by more than an order of magnitude.
- A concept similar to that employed by WISH at ISIS could be proposed using WFM. WISH is foreseen to implement PA and is mainly a powder instrument and is also designed to be able to study single crystals but has yet to produce definitive results.

2.2.6 Macromolecular crystallography

Science drivers

Biological macromolecules such as proteins and nucleic acids are involved in all biological processes and their function cannot be understood without knowing their structure at an atomic level. The most widely used method for macromolecular structure determination is crystallography, most often using synchrotron Xrays. Besides the contributions to fundamental science that have resulted in numerous Nobel prizes [17], macromolecular X-ray crystallography is also routinely used in the pharmaceutical industry to help develop better drug molecules. Neutron macromolecular crystallography (NMX) provides information complementary to that of X-rays – namely hydrogen positions – that cannot be obtained by other means. The potential user community includes the majority of X-ray crystallographers and is therefore very numerous. The hydrogen positions are of particular interest in investigating enzyme mechanisms where the protonation states cannot be inferred. The relevance of enzyme mechanisms is not limited to understanding the fundamental processes of life such as proton translocation [18], but also many drug targets are enzymes. A precise knowledge of the hydrogen positions is also important in drug design, as well as in engineering new enzymes for industrial use.

The widespread use of NMX has been limited by the availability of suitable instruments for NMX at existing neutron sources and their sample size requirements. Crystallographic data collection is essentially limited by the signal-to-noise ratio, which can be overcome by either increasing the size of the crystal or the brightness of the source. Due to the weak neutron fluxes available NMX requires very large crystals, which has been the major limiting factor. The crystal size required depends very strongly on the unit cell volume, since the overall diffracted power is inversely proportional to its third power. Commonly used crystallisation techniques for X-ray crystallography are not well adapted to growing such large crystals and therefore the majority of X-ray crystallographers find it daunting to grow such large crystal. Increasing the source brilliance or decreasing the background can obviously relax this limitation in crystal size, but larger unit cells can also be studied by adapting technologies that allow the large crystal growth to be optimised. While the time integrated flux of the ESS is comparable to the ILL, a brilliance gain is not evident, but the time structure of the source allows the Bragg reflections to be separated also in the time-of-flight dimension, which significantly improves the signal-to-noise ratio.

A long pulse source is particularly well-suited for an NMX instrument, since almost the entire pulse width can be used productively, which could provide two orders of magnitude performance gains compared to existing instruments. Such an instrument could revolutionise the scientific impact of NMX, allowing the study of a large number of systems that today are inaccessible with NMX.

Instrument concept

The existing instruments (LADI-III at ILL, PCS at LANSCE, iBIX at J-PARC, BioDiff at FRM-II, IMAG-INE at HFIR and MaNDi at SNS) are all built to cover a large solid angle by either a large cylindrical image plate detector or a polyhedral detector array, which effectively results in a fixed crystal-to-detector distance. This in turn means that there is an inherent limitation to the unit cell spacing that can be resolved for a given beam divergence and crystal mosaicity. The MaNDi instrument is capable of resolving unit cells up to 300 Å, but only at the expense of the smallest d spacing that can be measured ($d_{min} = 2.0 - 2.5$ Å).

A conceptually different design that resembles a modern synchrotron X-ray diffractometer is free of this limitation, however at the cost of increased data collection times for large unit cells. A bi-spectral moderator that provides high flux around 2.5 Å is ideal for macromolecular crystallography provided that the spatial and energy resolution is sufficient to separate the individual reflections. The required energy resolution can be achieved by a long (150 m) instrument, giving a narrower wavelength band compared (for example) to MaNDi. This has the added advantage of having fewer reflections in any one image, which makes the data easier to process. The required spatial resolution can be achieved by a large (50 cm \times 50 cm) area detector based on solid state semiconductor detection (EIGER/Pilatus type) placed on a 2θ swing to cover reciprocal space up to 120° scattering angle. This geometry provides good access to the sample position and allows additional detectors to be added to speed up data collection. In the case of smaller unit cells and strongly diffracting crystals the detector could be moved closer for faster data collection, without arbitrarily limiting the maximal size of the unit cell. The shorter wavelength of the incoming neutrons compared to existing instruments also reduces the number of crystal orientations required, as the "blind" area in the Ewald construction becomes smaller. Detailed Monte Carlo simulations will be performed in order to assess the relative performance of such an instrument, but it is likely that order of magnitude gains with respect to the existing instruments can be achieved.

The supporting facilities are crucial for the success of this instrument, particularly in crystallisation optimisation. This aspect is highly complementary with the needs of MAX-IV and an ESS crystallisation facility should be developed together with MAXLab.

2.2.7 Engineering diffraction

Science drivers

Structural integrity and materials performance. Over the last few decades, neutron diffraction has established itself as a unique and almost unrivalled tool for the non-destructive investigation of engineering materials, in particular metals. Dedicated beamlines for optimised materials engineering are now part of the instrument suite at every major neutron source. The applicability of the technique has attracted wide interest beyond the traditional materials engineers – it now encompasses fields as diverse as geology, ferroelectric smart materials and cultural heritage. The investigations can be undertaken both *ex situ* on static components in ambient conditions, as well as *in situ*, ranging from cryogenic to elevated temperatures, combined with simulated loading conditions, et cetera.

The technique has furthermore attracted significant interest and acceptance in industry, often contributing extensively to third-party funding of the facilities (for example, by selling beam time), although academicindustrial partnerships remain the norm. Beyond the ability to investigate micro-structural properties, the ability to accurately determine the triaxial residual stress fields inside large components is unchallenged by other techniques, such as synchrotron X-ray diffraction.

Neutron stress measurement is still the only neutron scattering technique that has been standardised to a pre-ISO level. While demand for stress measurements in manufactured components remains strong – in welded components in particular – the need for studying performance of materials and processes *in situ* is gaining ground. The growing demands on new materials and technologies – to be stronger, lighter and more environmentally friendly – makes ever more critical the need for in-depth understanding of the performance of new materials down to the atomic level, from martensitic TRIP steels to precipitation hardening aerospace aluminium and nickel super alloys. Additional needs include long time-base experiments on creep properties, requiring measurements only every couple of days, but with a high degree of automated sample handling.

The projected scientific needs are summarised as:

- 1. In-situ joining and processing.
- 2. Thermo-mechanical treatments.
- 3. Near surface measurements of the effects of surface treatments.
- 4. Deformation studies.
- 5. Large scale component stress analysis.
- 6. Combined macro-visualisation and micro-structural studies of components.
- 7. Investigations of irradiated materials.

Instrument concepts

Conventional instrument with pulse overlap option. The ESS long pulses provide high flexibility for this class of instrument, besides offering a high neutron flux that is superior or at least competitive with the

brightest neutron sources available down to approximately 1 Å. The "natural" length of the instrument is about 150 m, assuming a first chopper for pulse shaping. This is necessary, on the one hand, to access the relatively high wavelength resolution required, and on the other hand, to enable a well defined symmetric pulse shape. Such a configuration defines a single wavelength band of about 1.8 Å, but allows maximum flexibility in tailoring the instrumental settings to experimental requirements with the highest efficiency possible. In particular the chopper system can be specified such that:

- 1. The resolution can be chosen in a range from 1% to about 0.3%.
- 2. The resolution can be kept constant for the whole probed bandwidth, ranging from about 0.5 Å to at least 5 Å.

Various wavelength-frame multiplication and pulse-suppression schemes are being evaluated and will be compared to the results of a frame-overlap method, similar to the POLDI concept at PSI.

In summary, such a configuration allows the texture to be probed (if there is sufficient detector coverage), and allows strain investigations (90° detector banks), focusing either on a short wavelength range, covering a broad wavelength range consecutively, or covering a broad wavelength range simultaneously for kinetic studies. It even permits working with several overlapping bands in order to increase measurement speed, if a sample allows such an approach. Such a flexible instrument allows for the highest efficiencies for the broadest scientific cases, while at the same time posing no major technical or instrumental challenges. A detailed study of this concept is under way.

SPEED concept. The SPEED concept employs a highly-structured pulse cut out of the long pulse and relies on the fact that the materials studied have simple structures to deconvolve the data arriving at the detector. The concept is not new, but its application to a long pulse source is original. With optimisation it could significantly outperform instruments like VULCAN at SNS, although it remains to be seen how the data deconvolution process can handle more complex, non-cubic structures. At the heart of the instrument concept is the structured pulse (modulation) chopper, which determines the performance of the instrument. A prototype chopper is under development and will be tested in 2012 before the concept is taken further. The approximate instrument length would be 70 m, and the detector size of the order of 1 m × 1 m, with pre-collimation centred around a scattering angle of 90°. The $\Delta d/d$ resolution requirement is of the order of 2×10^{-3} with gauge volumes of 20 mm³.

2.2.8 Imaging

Science drivers

The application of imaging techniques in general and particularly also of neutron imaging covers a wide range of different fields [19] and hence the science drivers are quite diverse, that is a single science driver can hardly be defined. This is on the one hand due to the fact that conventional attenuation contrast imaging is a relatively simple technique that generally neither requires sophisticated sample preparation, detector geometries and environments and therefore does not significantly limit samples in size, geometry, material properties et cetera, nor does it depend on specific sample treatment, parameters and characteristics (magnetic, crystalline, liquid, et cetera), but complex objects and components are investigated as they are. The only limitations so far are that samples are suited by their composition and size to provide reasonable image contrast and that investigated structures or processes are on the scale of the resolving power of the imaging set up. On the other hand, and in addition to that, a number of novel methods became available in recent years that even extend the application range of conventional attenuation contrast imaging, by providing additional image contrast based on other material characteristics than just the attenuation coefficient. That these methods will profit from the ESS the most and that they can be integrated in one dedicated instrument will be outlined below. Some examples of highlight journal covers are shown in Figure 11.

Some of the most prominent application fields of neutron imaging nowadays are related to industry and cover quality assurance, failure detection as well as a large number of industry-related research and development projects conveying examples like investigations for automotive and aerospace components (engines, fatigue, particulate filters, bodywork), glues, concrete, fuel cell and battery technology and so forth. Such investigations very often do not produce (scientific) publications and are largely unseen. However, they have a financial impact, allow to employ people and/or to acquire equipment as well as to directly serve industry and society. In many cases, especially concerning R&D, such investigations are paralleled by academic research. This is well illustrated by the cases of fuel cell, battery, and hydrogen storage research and development.



Figure 11: Covers of *Materials Today* and *Nature Physics* featuring neutron imaging. Left: Hydrogen storage applications. Middle: Magnetic domains in a bulk crystal sample as seen for the first time with dark-field neutron tomography, published in Nature Communications in 2010. Right: Magnetic fields in bulk materials.

However, even when turning to science, the list of academic fields requesting neutron imaging is long and notably extends into humanities – here neutron imaging might be a singularity in neutron sciences. Historians, archeologists and palaeontologists as well as art historians rely on neutron radiography and tomography. Neutron imaging users also include biologists, agricultural faculties, geologists and many others [20]. Nevertheless the main focus is on material science, which is strengthened by recent developments concerning significant improvements in spatial resolution – today touching the 10 micron limit, after having started at 200 micron just a few years ago, and recently reaching out towards 1 micron – and on the other side by novel methods. Advanced neutron imaging methods are able to go far beyond conventional visualisation of the 3D attenuation coefficient distribution in complex samples and have the potential for spatially resolved investigations of crystallographic phases, crystal lattice strains and phase transitions, magnetic phase transitions, magnetic domains [21] and magnetic fields [22], as well as electric current distributions deep in the bulk of complex samples, 2D and 3D mapping of structural inhomogeneities beyond direct spatial resolution, that is reaching down into the nanometre range, to name only a few potential application of modern neutron imaging.

All these applications will profit enormously from the worldwide highest available time averaged neutron flux available for neutron imaging at the ESS. High (time averaged) flux is a precondition for achieving high spatial resolution as well as time resolution, which in turn can be predicted to be world leading at an ESS imaging instrument, and will thereby increase the attraction of neutron imaging for industry as well as for science even more than nowadays. In addition, while conventional imaging (using either a broad wavelength spectrum or monochromatic neutrons) will benefit only from the increased time averaged flux, novel methods and applications (like those in the previous paragraph) will take an outstanding advantage of the energy resolution provided by the time structure of the long pulse source. This can be foreseen to boost applications not only in materials science, but also in further methodical development where even more significant progress is to be expected.

It is these novel methods and the improvements in spatial resolution, both of which require a strong source and novel instrumentation concepts, such as provided by the long pulse source, that have the potential to significantly change the current science case of neutron imaging by shifting its weight more towards materials science, by increasing the feasible applications in this field strongly.

Flexible multi-purpose imaging instrument

A neutron imaging instrument is intended to serve both conventional imaging requiring mainly the highest available time averaged neutron flux, as well as a broad range of advanced methods profiting from wavelength resolutions of different orders of magnitude. This guarantees maximum attractiveness for industry as well as for science. However, this implies the search for novel instrumentation concepts in neutron imaging involving long neutron guides and a complex chopper system, as well as the need for imaging detectors that combine high spatial and time resolution. Advanced methods that require wavelength resolution, and hence specific attention in designing the instrument, are:

- Energy resolved imaging around Bragg edges in the attenuation spectrum of crystalline materials, which enables crystalline features to be addressed in imaging experiments and has been demonstrated in mapping crystalline phases, and micro-structural features as well as strain present in samples under investigation.
- Dark field contrast imaging that probes differences and inhomogeneities of internal structures beyond direct spatial resolution (that is $< 10 \ \mu m$) and provides access to the magnetic domain structure in the bulk of ferromagnetic materials.
- Polarised neutron imaging, providing the potential to gain information and enable visualisation of magnetic fields and electrical currents even within the bulk of massive samples as well as allowing for investigating samples on the basis of magnetic phase transitions, for example by mapping the Curie temperature distribution with 3D spatial resolution.

Basic boundary conditions and requirements. In order to achieve spatial resolution a pinhole geometry is considered the optimum solution for neutron imaging. Besides the distance between sample and detector, which should be kept as small as possible in any case, the size of the pinhole diameter, D, and distance to the sample, L, both limit the spatial resolution that can be achieved. Furthermore, neutron imaging requires a homogeneous (spatial, over the full utilised spectrum) beam cross section of reasonable size at the detector position. Sufficient and reasonable values for state-of-the-art instruments are $L_{max} = 10$ m and $D_{max} = 30$ mm, with a beam cross section at the detector of 25 cm \times 25 cm. The neutron transport will be optimised for these values, which define the divergence to be guided from the source to the pinhole. The requirements for wavelength resolution are quite diverse for different methods:

- 1. no wavelength resolution for conventional attenuation contrast imaging,
- 2. $\Delta\lambda/\lambda \simeq 10\%$ for dark field contrast imaging as well as Bragg edge imaging providing contrast due to micro-structural features,
- 3. $\Delta\lambda/\lambda \simeq 1\%$ for polarised neutron imaging to study magnetic field distributions and Bragg edge imaging focusing on texture-related investigation,
- 4. $\Delta \lambda / \lambda \leq 0.5\%$ for Bragg edge imaging providing strain maps.

Additionally, the wavelength range of interest differs depending on the application. However, the main range of interest can be identified to be from 1.5 Å to 6 Å, being extended by high resolution Bragg edge methods toward an optimum of 0.5 Å and by dark field imaging as well as polarised neutron imaging that are expected to also profit from measurements at significantly longer wavelengths.



Figure 12: Schematic sketch of a potential general layout of the multi-purpose imaging beamline.

Basic instrument design. The solution to realise both low and high wavelength resolution methods in one instrument with high efficiency, which cannot be done at a short pulse source, is to install a wavelength frame multiplication chopper system. Consequently the length of the instrument is defined in order to provide the lowest desired wavelength resolution of 10% for the shortest required wavelength for corresponding methods, that is about 2 Å. Together with the closest position for a chopper at about 6 m from the source, the burst time of 2.86 ms and the frequency of 14 Hz, the total length of the instrument has been chosen to be close to 60 m with the pinhole at 50 m from the source. A sketch of a possible layout is shown in Figure 12.

guide system between source and pinhole will include (at least) two focal points in horizontal direction, one at the pulse shaping choppers for WFM and one at the pinhole, while vertically one focal point at the pinhole seems to be sufficient. However, the guide system for the instrument with a given length and fulfilling the given requirements is still to be optimised. This includes eliminating direct lines-of-sight, in order to avoid gamma and fast neutron contributions that would impact the imaging quality, as well as a bispectral extraction system to provide reasonable flux at least down to a wavelength of 1 Å and its implications for the above.

The chopper system will consist of two pulse shaping choppers operating in an optical blind mode in order to enable constant wavelength resolution over the full bandwidth for all resolutions achieved by pulse shaping (in the range from $\leq 0.5\%$ to 1%). The triple-fold WFM implied by the source parameters and the instrument length is intended to be realised by discs with three individual windows optimised in width with respect to the specific wavelength frames, similar to the example of the chopper system layout at the ESS test beamline at HZB. The same applies to a number of wavelength frame overlap choppers (minimum two) guaranteeing to avoid overlap of the WFM subframes. Another frame overlap chopper will consist of two discs in order to adapt its opening time to whether or not the WFM is in place. The pulse shaping choppers will be installed such that the distance between them can be set to different values between 0.5 m (1%) and 0.2 m (< 0.5%) to tune the resolution. Their maximum speed (~ 8 - 10 times the source frequency), the set resolution and the shortest wavelength required define the needed focal width between them which will be realised by neutron optics (focusing and/or defocusing guide) and controlled by a slit between the choppers.

The flight path L between pinhole and sample position is evacuated in order to prevent air scattering, but with flexible elements in order to enable installation of additional required elements (gratings, polarisers, guide fields and so forth). Furthermore it includes a slit system in order to allow for beam collimation. The pinhole size can be decreased to any value below 30 mm diameter. An option to increase focusing accordingly has yet to be investigated. The sample position can handle a wide range of samples (size, weight) with high accuracy and several degrees of freedom in motion and needs to be accessible by a crane. The sample area is well equipped with gas, water and compressed air supplies, satisfying all requirements for standard sample environment equipment. The hutch around the sample position is spacious in order to handle big samples and equipment as well as active samples. Several imaging detectors will be available optimised for different resolution concerning time and spatial resolution. Further considerations include an X-ray source for complementary imaging investigations and finally the potential to install diffraction detectors, Engin-X-like for conventional strain measurements, and Imat-like for complementary texture investigations. (Engin-X and Imat are instruments at ISIS.)

White beam imaging instrument

It has to be expected that the imaging instrument – which allows for an outstanding variety of neutron imaging methods being applied with the worldwide highest available efficiency and the corresponding wide range of conventional as well as novel highly sophisticated applications – will be significantly overbooked and hence limited in flexibility in its schedule, in order to satisfy the needs of industrial applications. Therefore a plan for a second, more specialised, workhorse instrument has to be considered – for example for standard applications and industrial investigations that do not require the full flexibility of the first instrument. Such a beamline might be constructed in a more straightforward manner, similar to the state-of-the-art at current high flux reactor sources: a length of 20-30 m, a single frame overlap chopper, and no neutron optics. This might allow eventually for a slightly higher flux density and even an extended beam size.

2.2.9 Spectroscopy for fast dynamics

Science drivers

Technological advances have in recent years been made via the discovery of a plethora of functional materials. Functional materials alter their physical and chemical properties in a technologically relevant way, in response to a change in their environment such as, for example, temperature, pressure, electric or magnetic field or optical wavelength. Their behaviour can only be properly optimised through a thorough understanding of their dynamic and spatial correlations. The dynamical processes that are of interest often span wide ranges in time and energy scales. Neutrons can be used as an ideal tool to probe the dynamic and spatial behaviour via the dynamic structure factor $S(Q, \omega)$. Indeed, most of our knowledge of elementary excitations such as phonons or magnons in crystalline solids comes from neutron spectroscopy. The science drivers for neutron spectroscopy range over a multitude of disciplines, encompassing many of the natural sciences:

• Strongly correlated electron physics.

Quantum phase transitions with new classes of quantum criticality.

- Superconductivity.
- Lattice, charge, orbital and spin degrees of freedom leading to exotic states.
- Electron-phonon coupling.
- Frustrated magnetic behaviour.
- Molecular magnets.
- Topological materials.
- Functional materials.
 - Topological insulators.
 - Thermoelectric materials.
 - Nano-structured materials.
 - Carbon nanotubes.
 - Catalysts.
 - Intercalation compounds.
 - Hydrogen storage.
 - Solid-state ionic conductors for batteries, fuel cells and sensors.
- Disordered materials.
 - Liquids and glasses.
 - Collective behaviour in liquids.
- Soft matter and biophysics.
 - Polymer and biopolymer gels and membranes.
 - Confinement and targeted drug delivery.
 - Soft matter self-assembly.

Spectroscopy at the ESS will differ from its counterparts not only via the long pulse nature of the source but also via the comprehensive use of focusing optics to focus on small single crystals. It is only via the scattering from single crystals that we are able to obtain full spatial and energy information on exchange interactions. However, for many materials it is impossible to grow the large single crystals that are required for the current generation of instrumentation. Instruments at the ESS must therefore be able to extract information from smaller and more weakly scattering samples. In addition, many of the crucial inelastic experiments will be performed using extreme sample environments, such as high magnetic fields and high pressures to alter the fundamental properties of the materials. Such inelastic neutron experiments will be limited, not only by the inevitably reduced sample volume, but also by the decreased angular opening of complex sample environments. The instruments that we will build will therefore require highly optimised incident focusing optics, down to mm sample sizes.

Current state-of-the-art instruments for inelastic scattering include wide-mapping time-of-flight spectrometers at both continuous and spallation sources and point-by-point triple axis type spectrometers at continuous sources. Chopper spectrometers, in particular in the cold spectral regime, are ideally adapted to the source parameters of the ESS. Concepts derived from triple axis spectrometers can be used to optimise crystal optics for beam monochromatisation or energy analysis as further instrumentation concepts. The versatility of spectroscopic instrumentation in conjunction with advanced computational techniques will ensure that these instruments will have a great impact on many fields of study.

Chopper spectrometers

A range of instruments that, together, achieve a high energy resolution reaching 4 μ eV will realise an overlap with backscattering and spin echo spectroscopy. Furthermore a wide dynamic range 0.2 < E_i < 300 meV is needed to cover the broad range of scientific applications. The **Q** resolution should be tuneable from 0.005 to 0.15 Å⁻¹. The following technical areas are of primary importance for the development of chopper spectrometers:

- ³He-free detectors covering as much of 4π as possible.
- Variable focusing for small samples (down to $1 \text{ mm} \times 1 \text{ mm}$).

- Polarisation analysis using polarised ³He and/or supermirrors.
- Q resolution for single crystals: effect of guide and focusing.
- Achieving a homogeneous beam profile for co-aligned crystal samples.
- Ability to trade flux for resolution and vice versa.
- Energy resolution must be a simple function.
- Very high signal-to-noise ratio.
- Sample environments integrated into the instrument to minimise background scattering and to maximise beam optics performance and detector solid-angle coverage.
- Low angle coverage for magnetism.
- Full 3-dimensional polarimetry is currently only implemented for single detector instruments. The technique needs adaptation to wide angle coverage.
- Instrument must be non-magnetic to allow magnetic fields as a sample environment and polarisation analysis.
- Data analysis for wide $S(Q, \omega)$.
- Simulation and experimental results for the feasibility of Repetition Rate Multiplication (RRM).
- Event recording will ensure flexible data processing after the experiment is conducted.

Cold chopper spectrometer – concept 1: A cold high resolution chopper spectrometer that makes use of RRM to maximise flux [23]. This concept was studied by Lefmann *et al.* [24] and is currently being further developed [25]. The science drivers have not yet been fully defined but there are strong indications that the user community wishes to have very high resolution down to 4 μ eV, and to be able to reach incoming energies beyond 80 meV. At 150 m in length, the instrument can reach an energy resolution better than 1%-2% for wavelengths above 5 Å, while using the full pulse width of 2.86 ms [24]. Simulations indicate that the transmission of cold neutrons through elliptical guides is excellent and is preferable to a shorter guide with equivalent resolution obtained by a pulse-shaping chopper. Simulations of the beam profile through an elliptical guide show that divergence is not an issue – the brilliance transfer through an elliptical guide decreases from 1 at zero divergence to 0.95 at 2° divergence for a 150 m guide. One of the essential features of a chopper spectrometer is the ease with which it is possible to trade flux for energy and momentum resolution. The chopper configuration on the cold spectrometer must maintain this ease of variability.

The push towards smaller sample sizes (as small as 2 mm × 2 mm) will require focusing optics that can be translated or interchanged into the incident neutron beam. The divergence of the beam must be carefully simulated for such focusing optics. It is also important to match sample size to detector pixel size. Currently it is possible to achieve 10 mm × 10 mm pixel size. The importance of resolution versus sample size (and thus detector pixel size) needs to be evaluated. To obtain a good elastic resolution we consider a sample to detector flight path length of at least 4 m. The energy resolution function of the spectrometer will ideally be a perfect Gaussian line shape. In addition special consideration will be paid to the momentum transfer resolution for single crystal samples. A flat beam intensity profile for samples that are composed of several co-aligned single crystals is important when mapping $S(\mathbf{Q}, \omega)$ in all four dimensions. The implications of guide design and focusing for momentum resolution and beam profile will be considered. The most recent simulated example [26] of a cold neutron chopper spectrometer employs RRM with 9 monochromatic pulses on the sample. The neutrons are transported via an elliptical guide that focuses to 20 mm × 20 mm at the sample position. The instrument length is determined by a resolution input of 1.6% at 5 Å. This gives rise to an instrument length of approximately 120 m (source to fast chopper) with an instrument bandwidth of 2.2 Å (3.9–6.1 Å).

Cold chopper spectrometer – concept 2: A multispectral chopper spectrometer [25]. To extend the spectral range of a cold neutron spectrometer into the thermal range it is possible to use a multi-spectral extraction system. Recent simulations have shown that it is possible to combine cold and thermal neutron spectra with an efficiency of the order of 80%, when compared to a uni-spectral guide system. Further guide simulations are in process. Two concepts are under considerations, a wide bandwidth spectrometer for fast mapping (50 - 80 m) and a medium bandwidth spectrometer with flexible resolution (120 - 160 m). A design emphasis on large solid angle coverage, and on neutron energy loss scattering, leads to a sample-to-detector distance of approximately 4 m. Both instruments will make use of RRM with energy bandwidths chosen to represent the scientific needs of the user community.

Thermal chopper spectrometer: A dedicated thermal chopper spectrometer. The instrument will sit 200-300 m from the source, in order to focus the intensity into the thermal-neutron range. The principle will thus be similar to a cold chopper spectrometer using the full ESS time-frame, but made longer to optimise the thermal-neutron performance. The thermal neutron transport over 300 m has been simulated [26]), showing losses as low as 10% - 20%. This is possible with an elliptical guide with varying m values for the supermirror coating from m = 6 at the ends to m = 1 in the centre. The feasibility of this instrument lies in the cost of shielding and guides.

Crystal-monochromator chopper spectrometer: A thermal incident beam (10-80 meV) is monochromated by a crystal monochromator while the scattered beam is analysed by time-of-flight. A crystal monochromator can provide a large focusing gain on the sample, when compared to a supermirror-based device, especially at thermal wavelengths. The long pulse nature of the source will allow time focusing between monochromator take-off angle and chopper transmission time, by appropriate choice of the chopper rotation parameters. Time-of-flight measurements eliminate higher order contamination. This type of instrument is expected to be particularly interesting for the shorter wavelengths (with incident energies up to 80 meV). This instrument will resemble IN4 at the ILL, with the difference that the total flux in a pulse is collected and time focused using the crystal monochromator. Time focusing is thus adapted to energy transfer. The resolution will be governed by the monochromator design. Such an instrument would not be longer than 30 m.



Figure 13: Inverse geometry instrument for spectroscopy on small samples under extreme conditions. A single analyser channel is shown in detail, illustrating how several wavelengths can be analysed simultaneously by placing consecutive analysers behind each other.

Crystal analyser spectrometers

Concept 1: cold indirect geometry crystal optics spectrometers. The instrument shown in Figure 13 is for inelastic neutron scattering studies of small single crystals and is particularly optimised for extreme condition sample environments when the sample environments limit the vertical view to the sample. This is the case, for example, for experiments in strong magnetic fields or in pressure cells. The inverse geometry instrument combines a time-of-flight primary spectrometer with a multi-analyser secondary spectrometer. Receiving a polychromatic incoming beam, and measuring neutrons at many scattering angles into multiple energy bins, it approaches the theoretical maximum possible count rate of neutrons scattered in the horizontal scattering plane and preliminary simulations indicate significant gain factors over existing instruments with similar momentum (Q) and energy (ω) resolution [27, 28, 29]. A prototype will be built and tested at the PSI. This concept can also be used for a (sub) thermal instrument enlarging the dynamic range at the expense of resolution.

Concept 2: Crystal-monochromator spectrometer. Both the multiplexed crystal-analyser optics described above and the conventional time-of-flight secondary spectrometer can be combined with a primary spectrometer using a crystal monochromator. This might be advantageous to:

- 1. maximise the monochromatic flux on the sample, with
- 2. reduced background and sample activation with respect to white beam instruments, and
- 3. improved resolution control.

The time structure of the source will be used to separate the Bragg harmonics from the crystal monochromator. Phase space transformation in the primary spectrometer [30] will be studied to increase the intensity at the sample position for a limited wave-vector range.



Figure 14: Scientific areas that can be covered by the combination of the proposed spectrometers at the ESS. Adapted from J. Gardner, NIST.

2.2.10 Spectroscopy for slow dynamics

Following on from the discussion of fast dynamics, the observation of dynamic processes require a multitude of instruments to cover the wide dynamic range of molecular motions, from internal molecular vibrations to slow diffusion. Vibrational neutron spectroscopy is most efficiently carried out with an inverse geometry spectrometer using analyser crystals and wavelength filters, as seen on instruments such as TOSCA (ISIS), VISION (SNS) or LAGRANGE (ILL). In some cases the Q-dependence of the vibrational spectra needs to be explored with the aid of a high-incident-energy chopper spectrometer such as MARI (ISIS) or SEQUOIA (SNS). Low frequency molecular excitations, as well as fairly rapid rotational and translational diffusive processes, can be observed with a wide variety of instruments, mostly in direct geometry as described in the previous section, but also in inverse geometry such as the backscattering instruments IRIS and OSIRIS (ISIS). The latter instruments have a distinct advantage in terms of having high energy resolution over a wide range of energy transfers in energy loss away from the elastic peak, and at high Q.

Slower dynamic processes can be probed by higher-resolution backscattering instruments (IN16B at the ILL, SPHERES at FRM-II, BASIS at the SNS), while the longest timescales, reaching into the microsecond range, can be accessed by encoding changes of energy in the neutron spin, as performed in neutron spin-echo spectroscopy instruments such as IN11 and IN15 at the ILL and NSE at the SNS. The various regions accessed in momentum and energy space by these instrument types are shown schematically in Figure 14 together with indications of the scientific areas to be covered.

Science drivers

Scientific applications in this time regime can roughly be divided into two main areas of (Q, ω) space, namely low-frequency inelastic spectroscopy and quasi-elastic neutron scattering.

- 1. Low frequency inelastic spectroscopy.
 - Rotational tunnelling spectroscopy (H₂, CH₄, CH₃, NH₄, ...).
 - Hyperfine interactions.
 - Low frequency excitations in glasses (for example aerogels and fractons) and liquids (for example rotons in liquid helium).
 - Magnetic excitations, as in molecular magnets.
- 2. Quasi-elastic scattering.

Selected examples of processes observable by quasi-elastic neutron scattering and their relevance are:

• Diffusion on the atomic and molecular level.

Diffusion of hydrogen (H₂, atomic H, H ions), or Li+, in metals, alloys, or porous materials (for example for H-storage materials), fuel cells (understanding of basic transport in membranes), materials for fuel cell electrodes, battery materials.

Diffusion of atoms and molecules on surfaces in porous materials (gas storage) or in catalytic materials.

Proton transfer in hydrogen bonds.

Rotational diffusion (stochastic reorientation) of large molecules.

• Macromolecules.

Dynamics of polymers, polymer films and polymer blends.

- Nano-composites.
- Molecular rheology.
- Soft matter.
 - Complex fluids.
 - Micro-emulsions.
 - Phase transitions.
 - Confinement targeted drug delivery.
- Biologically-relevant systems.

Dynamics of biological or bio-related molecules.

- Protein domain dynamics.
- Nanosecond diffusion of proteins in aqueous solutions.
- Membrane dynamics.

- Magnetism.
 - Spin glasses and frustrated magnets. Spin ice. Damping of magnons. Dynamics of phase transitions, critical scattering.

Backscattering spectrometers

Backscattering spectrometers achieve high resolution by using single crystals with their Bragg planes aligned exactly, or very close, to perpendicular to the direction of the scattered beam. Both the time and spatial domains for many of the dynamical processes listed above are accessible to quasi-elastic neutron scattering using directgeometry spectrometers. However, backscattering spectrometers have the advantage of giving information over a wider range of Q, when compared with direct geometry instruments of comparable resolution. Thus, more details of the geometry of the motion are obtained. Depending on the prioritisation of the scientific requirements on energy resolution, bandwidth and Q-range, such an instrument might be up to 300 m long. As calculations indicate that efficient neutron transport is possible over very long distances, the instrument length will mainly be limited by the cost of the long guides and the associated shielding.

Concept 1: Backscattering spectrometer with high and variable resolution. A backscattering instrument with variable energy resolution in the μ eV range is envisaged, in order to facilitate investigations extending over a dynamic range of accessible energy transfers that is greater than currently possible at other neutron sources. A flexibly conceived and designed neutron backscattering spectrometer can cover a wide range of time and length scales in between those probed with time-of-flight chopper spectrometers (TOF) and spin-echo experiments.

Concept 2: Backscattering spectrometer with a high resolution of 2 μ eV. A very straightforward realisation of a backscattering spectrometer would be similar to the BASIS spectrometer at SNS, providing an energy resolution of the order of 2 μ eV at the detectors. The scientific capabilities of this instrument would be complemented by spectrometers at European reactors and at international spallation sources that offer resolutions of less than 1 μ eV. It is however expected that a high-resolution backscattering instrument would cover an extended dynamic range, of the order of 500 μ eV. This instrument would also allow for comparison with predictions from molecular dynamics calculations involving longer length scales, which in turn require an increase of the corresponding timescale – that is, higher energy resolution – for their observation.

Neutron spin echo

Neutron spin echo spectroscopy is the technique with the highest energy resolution. While no comprehensive review has yet been carried out amongst the European science community, it is still clear that for neutron spin echo spectroscopy there are a number of key areas that should be addressed:

- Intensity is always a key requirement in NSE, particularly for small samples or dilute difficult samples. One method to increase the effective flux is to improve the solid angle coverage achievable. The challenge would be to develop suitable field homogeneity correctors.
- Focusing for small samples while maintaining the field integral.
- Expanding the available (Q, τ) range is also highly desirable. This includes the ability to measure to lower Q, but at high Fourier times (interesting for soft matter and complex fluids), but also to expand the available timescale into the sub-picosecond range, so that the full dynamic range can be covered by one instrument.
- Magnetic samples are always a challenge for NSE since magnetic domains depolarise the neutrons. This is also true for measurements in magnetic fields. Therefore it is necessary to decouple the magnetic sample fields from the precession fields and to have a special setup in the sample area. This might be achieved using the MIEZE (NRSE) technique [31].
- NSE requires high stability in terms of electrical (current) fluctuations, mechanical instabilities (thermal expansion) or external influence from magnetic fields (cranes, neighbouring instruments). This is a particular requirement for many sensitive science problems such as subtle effects in protein and polymer science.

- Comparison of normal and superconducting coils. Performance of magnetic screening concepts
- Separation of coherent and incoherent scattering intensities. At high momentum transfer, the intensity of the coherent signal drops below that of the incoherent (background) signal, typically with differing contributions to the dynamics. Currently, the only solution is theoretical modelling or measuring with different mixing factors. MIEZE is one possible practical solution.
- Ample space for specialised sample environments is needed. Excellent temperature control is desired with at least 0.01 K accuracy. The ability to apply external stimuli (fields, shear) and the possibility to do magnetic field measurements very close to the sample.

Concept 1: High resolution spin echo spectrometer. This instrument is currently being optimised for the ESS source parameters [32]. It will obtain very long Fourier times (up to 1 μ sec) by using long wavelengths and new concepts for resolution enhancement. Most likely employing a solenoid geometry for the precession coils, the instrument must be placed fairly close to the source and on the outer edge of one of the neutron beamline sectors in order to maximise the dynamic range.

Concept 2: Wide angle spin echo spectrometer [32]. Optimised for the 4-12 Å wavelength range and covering a very large solid angle, giving the largest gain factors for incoherently scattering samples. A large area of polarising supermirrors and detectors will be required.

Concept 3: TOFLAR. This instrument concept has been developed by the NSE group in Delft, and proof of principle performance has been reported [33]. The energy of the incident beam is encoded using the precession time of a neutron in a magnetic field via a Polariser/Coil/Analyser assembly. The energy of the scattered beam is determined using TOF. The technique enables inelastic and quasi-elastic measurements in the nanosecond to picosecond time domain. This concept can either be used as an add-on for a neutron spin echo or MIEZE instrument or can be a stand-alone instrument for quasi-elastic scattering with high intensity but medium resolution.

Concept 4: A high resolution spectrometer using the MIEZE technique as high resolution Larmor encoding of the neutron velocity [34]. The concept involves time-modulating the intensity of the incoming beam. This technique is well-suited for the investigation of magnetic samples or investigations on strongly incoherent scattering probes because the entire beam preparation takes place in front of the sample. In addition, the setup could be placed as an option for small angle scattering instruments. A proof-of-principle experiment has been performed [35] and the application for small angle scattering has been elaborated [36].

Further concepts: Auxiliary measurements. SANS measurements on an NSE instrument would be of particular interest for samples with a limited lifetime such as proteins. It would require the intensity to be measured without the dynamics analysis, but with polarisation analysis, and a wide Q range with reasonably low Q resolution.

2.2.11 Hybrid instruments

Science drivers

Hybrid instruments are those that are not optimised for a single class of measurement (for example diffraction or imaging) but where multiple measurements are performed (for example simultaneous diffraction AND imaging measurements). Other examples include combined elastic and inelastic measurements to simultaneously probe structure and dynamics, and a combination of elastic measurements – such as diffraction and/or SANS – with real time direct space measurements – such as imaging – where simultaneous information on multiple length scales is required. The basic science case mirrors those in the sections on diffraction (both powder and single crystal), SANS and imaging, but are focused towards topics where repetition of conditions by performing separate experiments is difficult or impossible. A second type of hybrid instrument has a complex sample environment geometry that compromises the available scattering angle to such an extent that it is preferable to build an instrument around the sample environment, rather than to modify the sample environment to fit into an existing instrument. Examples of complex sample environment are the traditional extreme environments, such as pulsed magnetic fields and pressure cells, although this can increasingly be extended to include reaction cells, gas chambers, humidity cells, deformation rigs, et cetera.

The technological impact in these areas has seen a marked rise in the last decade and neutron sources have moved towards dedicated instrumentation for extreme sample environments (for example SNAP at SNS, EXED at HZB, PEARL at ISIS, and PLANET at J-PARC). Fast diffraction instruments, such as D20 at ILL and POLARIS at ISIS, have made significant impacts in *in situ* chemistry and processing, but are not optimised for the restricted geometries or sample sizes imposed by the sample environment and must compromise in some way to perform the experiment. It is clear that optimising an instrument around a sample environment that is more suited to the chemistry world would have a high impact in the user community, as long as parallel efforts are made in collaboration with the user community to develop the sample environment alongside the instrumentation.



Figure 15: Proposed time structure use and instrument layout using a dual cold and thermal guide system [37].

Diffraction/SANS/imaging. The goal of this hybrid instrument is studying materials *in operandi* and *in situ* at multiple length scales using high resolution. The concept is presented briefly in Figure 15, while Table 5 summarises the length scales for each technique. The major challenge is combining the different methods optimally in a single instrument. The diffraction instrument would be based on the narrow bandwidth concept previously described using a thermal guide and be around 150 m long with a wavelength band of 1.8 Å. The cold guide would be used for SANS, cold neutron powder diffraction and imaging. The proposed instrument alternates the pulses from the thermal and cold guides in a 4:1 ratio in order to obtain the extended bandwidth required for SANS at the same position as the optimised thermal diffraction guide. Cross-talk from the thermal neutrons into the SANS detector would be reduced by a beryllium filter. Considerable further effort is required to find a workable solution.

Technique	\mathbf{Units}	Length scale range	
Diffraction	nm	0.01 - 5	
SANS	nm	1 - 1000	
Imaging	$\mathbf{m}\mathbf{m}$	0.01 - 100	

Table 5: Summary of the length scales probed by the different techniques.

Diffraction and/or imaging for extreme conditions. This instrument would be optimised to be able to support a broad range of *in situ* experiments using complex sample environments. This requires compromising the 'ideal' detector arrangement for a diffraction instrument in order to give access to the sample position in order to accommodate the wide range of user supplied cells. The design also allows secondary measurements to be performed, such as direct imaging, due to the reduced detector coverage. Restricted detector geometry could be mitigated by strong vertical focusing of the guide, allowing sample size to be reduced ($< 10 \text{ mm}^3$)

opening up the spectrum of sample environment more often seen at the current generation of synchrotron X-ray sources. The expansion of complementary X-ray and neutron *in situ* measurements would be highly desirable to the user community. A basic layout of an instrument is given in Figure 16, based on a narrow wavelength band setup.

Instrument summary:

- Medium resolution powder diffractometer combined with imaging ($\Delta d/d$ from 0.15% in backscattering to 0.5% at 90° for small samples).
- Split detector system allowing access to sample position.
- Combined angle-dispersive, time-dispersive data collection.
- Variable resolution detectors.
- Can perform strain measurements.
- Could profit from bi-spectral incident beam for diffraction and Bragg edge imaging.
- Polarisation of incident beam possible.
- Able to accommodate high field magnets with restricted geometry.
- Adjustable apertures in final 20–30 m section of guide to reduce beam divergence and to shape beam for direct imaging measurements.



Figure 16: Proposed layout of the diffraction and/or imaging instrument.

2.3 Science support

The ESS will be part of the future suite of European research infrastructures providing experimental possibilities to research from both academia and industry. For its scientific success, the ESS has to be governed by scientific needs and this goal determines the outline of this section on "Science support". On the current level of detail the resulting requirements are robust but will need to adapt at a later stage depending on the policies adopted concerning the following aspects:

- 1. User access modes (both proprietary and public) including in-house research.
- 2. Intellectual property and data ownership.
- 3. Scientific collaboration, education and outreach.

In the current situation, emphasis is put on scientific motivation and defining interfaces and requirements.

2.3.1 User programme and academic activities

For a successful neutron science user programme different access modes have to be considered. Such a user programme will provide a path to answers of scientific questions, not just beam time. For this, reliability of the source and also in the measurement itself is essential. User input will be gathered through meetings, feedback, and industry days to refine continuously the user's needs.

The large majority of research will be public non-proprietary research. The user programme will ensure free access to the research facilities covering the costs for the researchers coming to the ESS. A peer review proposal system ensures transparency and equal access to the research facilities. Scientific merit and feasibility will be the prime selection criteria. Secondary aspects, such as national balance, publication record as well as training will be considered. More sustained project based work will also be considered in addition to the conventional experiment-based proposal system. To ensure maximum success rates, the project selection has to be structured by topic, and might consider complementary measurements at other facilities. In addition to the basic experimental requirements (instrument and technical support), requests for additional resources prior to and after the experiment and evaluation of training needs will be considered. Provision for test experiments at the ESS and elsewhere has to be explored to maximise success and ensure efficient use of beam time. The ESS will be important to industry by offering a unique, cost effective tool for targeted, strategic research in the development of novel materials, processes, controlling emerging technologies or exploring future research avenues [38]. Industrial research is performed either as proprietary or public research, the latter through academic partnerships. A dedicated "industry liaison office" will support the industry-related activities, both public and proprietary, ensuring adequate access modes and support facilities. Proprietary research especially requires an emphasis on intellectual property rights, confidentiality, accreditation and certification. In-house research is essential to the credibility of the ESS and its scientists. To this end, provision for flexible rapid access time will also be important to rapidly adapt to scientific swings. Instrument test time will be set aside to ensure continual experimental equipment (instrument upgrades, add-ons, and auxiliary equipment). To be effective, all such activities require reporting and (internal) review. The in-house activities determine the focus of the on-site support labs as well as the student programme. Access to academic resources is required. Independent of the user access mode, the needs to provide facilities for the whole user experience such as on-site workspace (office, network access, library) networking (meeting rooms, coffee machine) accommodation (guesthouse) catering (canteen), recreational possibilities (gym). Rapid commuting within the scientific site (ESS, Max-IV, Lund University) is required.

To ensure a wide scientific breadth and sustainability in neutron research, outreach and education is important. This includes student programmes open to collaborating European partners and strongly involving the local scientific community. These training activities require conventional facilities (lecture hall, seminar rooms), on-site human resources and coordination within the ESS.

2.3.2 Sample handling and support labs

The performance gain of the ESS will not only allow faster experiments (higher throughput) but also experiments on more challenging samples. Using available (potentially smaller) samples enables the ESS to provide results in the stream of research performed at university and industry. For an efficient and successful use of beam time, many samples will have to be prepared or conditioned on-site using adequate facilities. The cost for such support equipment is small compared to the huge investment made towards the facility. It is, however, important to distinguish between what should be done at the home institutions and what the ESS should provide in order to guarantee successful neutron experiments. Since beam time is a precious resource, it is important to help users to ensure that the measured sample has the expected characteristics and has not, for example, been damaged during travel. The facilities will complement those available at the home institute or at the specialised local infrastructure. The facilities will take the special requirements of neutron samples (isotope substitution, special containment) into account. Neutron test beamlines for instrument development but also scientific feasibility studies will be investigated.

Safety is of utmost importance and samples have to be handled safely before, during and after the experiments. Potential risks will be taken into account such as radioactive material, biological and chemical hazards as well as toxicity. Appropriate and safe handling are prerequisites for a successful research project. Waste disposal for both nuclear and conventional waste has to be established and zoning should be planned so as to ease sample handling between the various labs. Given the size of the facility and the distances involved, logistics and infrastructure (pathways) have to be provided ensuring transport of sample, equipment and users.

The technical support required prior to and during a user visit is related to a specific experiment. For this, workshops are required close to the instruments. Mechanical workshops and technical capabilities are required to prepare items in a timely manner for running the user programme. The necessary lab facilities in the controlled areas all provide the possibility to condition the samples promptly before the experiment by an adequate number of users. Such facilities include sample handling, preparation and storage. Temporary storage of samples in adequate conditions will be provided.

User laboratory for biology. Separate biology laboratories are needed for working with cell cultures and biologically active materials, which require specific biosafety measures to be followed. The laboratory will be equipped with basic biochemistry equipment for the handling, separation, purification and characterisation of biological samples, as well as facilities for the growth and storage of biological crystals. The laboratory will be shared. The laboratory for biology will contain chromatographic equipment for last minute purification of samples. Crystallisation facilities for the controlled optimisation of large macromolecular crystals will be available.

User laboratory for soft condensed matter. A certain degree of sample fine tuning for soft condensed matter will be possible onsite in a dedicated laboratory. Soft matter laboratories outside the controlled area will contain all basic chemistry equipment required for handling, mixing, formulation, purification and separation of primarily organic but also inorganic and biological samples (which do not require specific biosafety regulations to be followed). They will not include facilities for chemical synthesis, however. While a significant fraction of the samples are aqueous solutions, the laboratory still needs to be equipped with fume hoods, chemical storage and disposal, cleaning facilities. It is extremely important that the laboratory has direct access to ultra-pure water. A laboratory for soft condensed matter will include basic equipment for the characterisation of sample density, concentration, morphology, et cetera, using a densitometer, UV-VIS and FTIR spectrometers, dynamic and static light scattering, Quartz Crystal Microbalance (QCM-D), an X-ray reflectometer, centrifuges and dialysis kits.

Deuteration facilities. Deuteration is an essential part of all soft condensed matter and biology experiments, and will be provided to all users. Deuteration will cover both biological and chemical deuteration, as well as facilities for purification, recovery and recycling of the biomass and/or chemicals. The methods and facilities needed for the chemical synthesis and biological expression are completely different and thus, essentially two separate facilities are needed. For efficient synthesis and expression of large quantities of deuterated samples, both will require large scale reactor and/or fermentor systems. The characterisation methods needed by both facilities will be shared, and will at minimum include NMR spectrometer(s) suitable for both small and macromolecules, LC-MS-MS for purification and characterisation of both small and macromolecules, HPLC for purification of macromolecules in aqueous media, HPLC for purification of small organic compounds in chemical solvents, densitometers, UV-VIS and FTIR spectrometer and plate reader as well as BiaCore or similar high throughput SPR for verifying the activity and/or function of deuterated samples. CD spectrometers as well as lab-sized SAXS machines will be considered.

Chemistry laboratories. Well equipped chemistry labs will be used not only for *ex situ* sample preparation and conditioning but also to supply support for the *in situ* equipment on the instruments. Besides fume hoods and bench space for preparing samples, there must be a dry glove box and an inert atmosphere glove box that can take liquid samples. Equipment includes four-decimal balance, density measurement apparatus, pellet press and associated dies, standard and/or vacuum drying oven, humidity generators and furnace capability (1200 C) with flowing gases (nitrogen, oxygen, helium, argon, and hydrogen). Sample characterisation requires access to a laboratory X-ray machine (various anodes) for powder checking. The chemistry labs might accommodate some of the equipment for bulk characterisation such as calorimetry TGA/DTA/DSC.

Laboratory for hard-condensed matter, crystallography and surface science. Due to its sensitivity to both magnetic and structural properties, hard condensed matter physics has been and still remains a core business for neutron scattering. Due to the different energy scales governing the properties of the sample, requirements for extreme conditions (temperature, magnetic field, pressure) are significant. Neutron experiments often require in situ measurements of magnetic and other electronic properties to link the results together. To prepare those, but also for supplementary ex situ measurements on the same samples prior to and/or after the neutron experiments, a dedicated hard condensed matter lab is required. Here some of the sample environment for extreme conditions (temperature, magnetic field, pressure) will be used. The laboratory needs to contain basic measurement equipment for magnetic susceptibility, specific heat and NMR observations. The equipment has to be compatible with the sample environment used on the instruments. This lab will also need to provide equipment to cut orient and co-align samples. This requires (hard) X-ray crystallography equipment to ensure the bulk of the (sizeable) neutron sample is probed. Co-alignment might be (semi)-automated using robotics. Not only glueing, but also bonding might be used to mount the samples. Inorganic thin films and multilayers need to be prepared for surface science using neutrons, but also as basic substrate for organic materials especially soft-condensed matter. Scanning tunnelling and atomic force microscopes will be considered, to complement the equipment in the other labs and to establish the domain distribution and/or homogeneity. Different light scattering apparatuses, such as Raman, IR, UV-VIS as well as pump probe techniques, are essential to complement neutron spectroscopy.

Facilities for actinides and highly radioactive samples. Actinide-based samples, special isotopes and highly activated samples will need to be handled in dedicated laboratories, enforcing approved handling procedures. Preliminary equipment includes glove boxes, equipment leak testing, sealing and/or encapsulation and dedicated storage space.

Facilities for engineering, geo-science and cultural heritage. Material scientists, geoscientists and cultural heritage scientists from both public and private institutions will require engineering facilities to handle, in this case, bulky real world samples. Equipment might include 3D measurement systems, welding and deformation equipment. Provisions for cultural heritage research will be made.

2.3.3 Local research infrastructure and scientific networks.

Users from both industry and academia might also want to profit from the inspiring environment of the ESS and Max-IV beyond sporadic experiments, in addition to the facility based essential infrastructure. Various possibilities exist to involve such a community. Several research topics require expertise available at only a very few institutes worldwide. A partnership could be envisaged with these institutes, creating a joint facility between the ESS, Max-IV and the expert partners. To ensure a long term perspective, budget from all partners have to be ensured. Those partnerships will be responsible for the topical user programme at the ESS and Max-IV. Several partners might want to profit from the benefits of proximity to have a long term outstation close to the ESS. Even though such a facility could run its own user programme and accept collaboration and visitors on a specific research topic, it would not have any responsibility nor cost towards the ESS user programme. For user communities looking into a mid-term involvement within the local scientific environment, local or regional universities could collaborate to provide a scientific home for researchers with collaborative research projects.

It should be reiterated that all activities have to be science driven. In this respect, the focus should not be on the facilities and the infrastructure but on the underlying vision. The scientific life created by the various different facilities and units will unfortunately not only be held together by an inspiring collaborative scientific exchange, but requires formally linking the various infrastructures – with their different funding, management and legal structures – to a science driven academic institute placed in the proximity of the ESS and MAX-IV ("Science City"). The ESS will take the lead and investigate from the beginning how its infrastructure can (logistically) integrate into this network, considering the various architectural, administrative and legal challenges. European scientists within such a network will more easily find the technical and scientific support beyond the scattering technique typically offered at existing neutron and X-ray sources [39].

2.4 Instrument support

The Instrument Support Division within the Science Directorate of the ESS is the technical division that supports the construction and operation of neutron instruments, and which will, in close collaboration with the European partner laboratories, develop specific hardware to ensure that the neutron instruments at the ESS will not only be, but will remain, state-of-the-art. At the present time it is anticipated that the Division will eventually consists of five individual groups, namely:

- Detectors
- Choppers
- Neutron Optics (including polarisation)
- Sample Environment
- Electronics and hardware units

The choice or definition of the groups follows the experience gained at other facilities, in particular next generation spallation neutron source such as the Spallation Neutron Source (SNS) at Oak Ridge, Tennessee, U.S.A. [40], the Japanese Neutron Spallation Source (JSNS) at the Materials and Life Science Experimental Facility (MLF) in Tsukuba, Japan [41] and the ISIS neutron spallation source at Didcot, UK [42]. In order to be able to support the Instrument Division it is necessary that the Instrument Support Division grows and develops expertise, while the neutron scattering instruments are being designed and subsequently built, that is, from early 2013 until 2025. Sufficient staffing levels are critical to successfully construct, commission and operate the neutron scattering instruments; they are also indispensable for efficient routine maintenance during shutdown periods or, and even more importantly, for unforeseen mechanical issues that could impact on the availability of the instruments during normal operation. At the same time the groups should have the right infrastructure in place to be able to service, develop and improve hardware used at the instruments such as detectors, neutron optical components or chopper systems to ensure that the ESS and its instruments are at the forefront of not only science related to neutron scattering but also the technology that enables high profile experiments to be carried out at the ESS.

2.4.1 Detectors

New kinds of neutron detectors, not based on ³He, are urgently needed, due to the very limited availability of ³He. For this reason the detector group was the first instrument support group put into place, in July 2010. Good progress on the Research and Development has been made since then, however the R&D will be ongoing past the end of the Design Update Phase, and into the Construction Phase. Currently the detector group consists of 4 members, including a research engineer in a joint position with MAXLab in Lund, whose main responsibility for the ESS will be in building up the detector laboratory. The aim of these collaborative links is to build up a core of competence in the Lund region for the necessary detector development.

The Helium-3 Crisis. In the last few years the demands for ³He have increased, mainly due to U.S. Homeland Security programmes, which in the past five years have used 85% of the U.S. supply. After the end of the Cold War, the production of this rare gas is very limited due to its main source being the radioactive decay of tritium [43]. This has led to unaffordable prices, especially for users outside the U.S. [44], and an urgent need for alternatives to ³He-based neutron detectors for large scale neutron research facilities [43, 44, 45]. The need is especially critical for new large area neutron detectors, which until 2015 will require more than the complete U.S. supply of ³He [43, 44]. The requirements for the ESS instruments were not included in these estimates and would significantly increase this demand further. Recently the situation has eased slightly for U.S. based users, with a limited supply being made available, although this is not expected to significantly change the situation for European users. The present market price in Europe of ³He, when available, is in the region of 3−5 k€ per bar-litre. This puts ³He out of scope for any future request, for large and medium area neutron detectors. This dilemma was recognised by the neutron research community in 2009, and led to the formation of the International Collaboration for the development of Neutron Detectors to investigate and develop alternatives. In particular, three Joint Research Activity (JRA) working groups were formed:

- 1. on ¹⁰B thin films (in which the ESS is centrally involved),
- 2. on BF_3 gas detectors, and
- 3. on overcoming the present drawbacks for scintillator technologies.

The ESS does not foresee building any ³He detectors in-house: any requirements for ³He detectors will be met from parties with the appropriate expertise already available, and who already supply the community with these detectors, such as institutes like Institute Laue Langevin (ILL), or commercial companies.

Detector requirements for the instruments. The estimated detector requirements from the 22 neutron scattering instruments outlined in this document are summarised in Table 6.

Instrument		Resolution	Pixel
	1 21	r 1	count
	$[m^2]$	[mm]	$[10^{3}]$
Cold chopper spectrometer	80	10	2.4
Narrow bandwidth powder diffractometer	30	2	6.5
Small sample SANS	1	1	0.2
Horizontal sample reflectometer	0.5	1	1.2
Macromolecular diffractometer	10	2	0.3
Multi-purpose imaging	0.5	0.1	15.0
Crystal analyser spectrometer.	1	10	0.2
Magnetism diffractometer	15	5	14.0
High resolution spin echo	0.3	10	0.13
Wide angle spin echo	3	10	0.35
Backscattering	0.3	10	0.13
Bispectral chopper spectrometer	50	10	1.2
Fundamental physics beamline	0.5	0.1	
Vertical sample reflectometer	0.5	1	1.2
Conventional SANS	5	10	0.45
Grazing incidence SANS	5	10	0.45
Thermal chopper spectrometer	20	10	1.0
Extreme conditions spectrometer	1	10	0.2
Extreme conditions diffractometer	10	1	6.0
General purpose powder diffractometer	30	2	6.5
Hybrid diffractometer with SANS & imaging	10	1	3.0
SPEED engineering diffractometer	10	1	2.0
Test beamline	1	10	0.2
TOTAL	283.6		62.61

Table 6: Estimated detector requirements for the 22 baseline instruments and test beamline in terms of detector area and resolution. The number of readout channels that will be required is also indicated.

Technologies chosen for R&D. Research effort has initially concentrated on large area detectors with $> 10 \text{ m}^2$, and with moderate requirements on resolution. ¹⁰B has been chosen as a possible absorbing element in a new generation of neutron detectors. The ESS is planning to build a demonstrator for a large area neutron detector with the IN5 gas detector at the ILL as a benchmark [46]. The detector will contain aluminium blades that are coated with ¹⁰B₄C layers where ¹⁰B absorbs the incident neutrons by the nuclear reaction

$$^{10}\text{B} + \text{n} \rightarrow ^{7}\text{Li} + {}^{4}\text{He} + 2.3 \text{ MeV}$$

Both the ⁷Li and ⁴He ions can be detected, with both temporal and spatial resolution, in a detecting gas. A full scale area detector is supposed to have an active surface of $> 30 \text{ m}^2$, which corresponds to $> 1000 \text{ m}^2$ of ¹⁰B containing thin films. For such a neutron detector to be competitive to the ³He-based detectors used today, high quality neutron converting thin films are important components. ¹⁰B₄C was chosen as the thin film material instead of pure ¹⁰B, because it is easy to handle in a deposition process like dc magnetron sputtering. B₄C is also well known to have excellent wear resistance, and thermal and chemical stability [47]. Based on the simulation results shown in Figure 17, we have investigated a process for growth of B₄C thin films using dc magnetron sputtering in an industrial deposition system. This deposition technique was chosen because it scales up relatively easily, incorporates little impurities, does not require very high deposition temperatures, and allows for high deposition rates.



Figure 17: Simulated parameters for optimal ${}^{10}B_4C$ thin film parameters to maximise the neutron detection efficiency, showing the effect of (a) layer thickness for 30 layers, (b) varied number of layers for 1 μ m layer thickness, (c) changing the neutron wavelength for 30 layers of 1 μ m thickness, and (d) adding 10 at.% of typical contaminants to 30 layers of 1 μ m thickness.





Figure 18: Top: Prototype boron-10 detector under test on the CT2 beamline at ILL. Bottom: Measurement of efficiency and neutron absorption as a function of depth. The red circles show the expectation from the simulation, while the black and magenta crosses show the measured values from two complementary methods.

Collaborations and joint ventures. A collaboration between ILL, ESS and Linköping University on boron-10 thin films recently successfully completed a ³He-free prototype detector ($2 \text{ m} \times 10 \text{ cm}$ active area with 30^{-10}B conversion layers, each 1 μ m thick). A test on the CT2 beamline at ILL successfully proved the feasibility of constructing and assembling such large area detectors. The experimental performance of the detector agreed well with simulation predictions, with a detector efficiency of about 50% for neutrons with a wavelength of 2.5 Å, as shown in Figure 18.

The next step is to scale up the current system to a full scale demonstrator with improved efficiency. The only thin films available for this second prototype are those produced by the ESS collaboration with Linköping University. The precision aluminium "blades" are sourced locally, building knowledge about local suppliers. The coatings for a recent 24/7 production run used only 10 of the 14 days available on the deposition system, and produced 5 m² of double-sided coated aluminium, significantly more than the 3 m² required. This is especially important considering the amount of area that will be required by the neutron scattering instruments at the ESS. The collaboration with Linköping University also enables trials to take place depositing boron carbide thin films through chemical vapour deposition. These are encouraging, although chemical vapour deposition is not the preferred method, due to the high hydrogen content of the film. It may also be possible to deposit stable GdN thin films by sputtering, a potentially useful future avenue.

Detector laboratory and thin films venture. A tripartite collaboration between the detector group at the ESS, the Nuclear Physics Group at Lund University, and the Photo-Nuclear Group at MAXLab will establish a joint detector laboratory, allowing detector development to start locally in Lund. This important step for the prepare-to-build phase will also bridge the gap until a detector laboratory is available on the ESS site. The detector group has significant contributions from Germany, Norway and Italy. Initial contacts about a possible contribution from the Czech Republic have been made. Also under investigation is a way to set up a thin films spin-off from the successful R&D work on enriched ¹⁰B thin films performed in collaboration with Linköping University. The initial scope will be thin films needed for the detectors. If successful, the scope may be expanded to cover other thin film requirements, in particular neutron optics, such as the coatings for guides. This model may also serve as a possibility for detector production. Detector systems using other techniques (besides the ¹⁰B thin film approach) are also currently under investigation.

Scintillation detectors using ⁶LiF-ZnS in combination with wavelength shifting fibres. A special focus is on large detection areas and a high conversion light output. Scintillation detectors were to a great extent pioneered at ISIS and they are particularly well-suited for thermal neutron scattering applications. A concept developed by FZ Jülich [48], which aims at improving the resolution attainable by using x - y meshes, is shown in Figure 19.

Anger cameras. Current prototypes developed in Jülich [48] typically have an active area of 100 cm^2 using 64 multi-anode photomultiplier channels, thus increasing the number of pixels per area. The development is aimed at optimal resolution performance. The principle is demonstrated in Figure 20. Two aspects are key to this design to be able to fully utilise the concept:

- 1. controlling the aspect ratio between the scintillator area and the PMTs and
- 2. being able to calibrate the gain in signal response between and across PMTs.

Gas electron multiplier detectors. GEMs have the advantage of high rate capability (up to MHz/mm²), extreme spatial resolution and relatively cheap costs. The difficulty for neutron detection lies in optimising the efficiency for the conversion layers, which could either consist of ¹⁰B or Gd, on the foils. GEMs are considered as suitable detectors, for example, for tomography or for radiography applications.

Gd-Micro-Strip Gas Chambers. The R&D for Gd-MSGC detectors, as shown schematically in Figure 21, is carried out at Helmholtz Zentrum Berlin [48]. MSGCs were originally developed at the ILL and first used on the D20 instrument at the ILL. They have also been used in other fields, including being the original proposed detectors for the tracking detector for the CMS experiment at the LHC. The detectors proposed here consist of a gadolinium conversion layer of $0.5-1.5 \mu$ m thickness, where the electrons emitted as part of the conversion (80% probability) are further amplified by a CsI layer immediately on top of the Gd layer. The electrons then enter a gas mixture (such as isobutane or Ar/CO₂), and the subsequent ionisation of the gas is detected on a microstrip plate. The microstrip plate has x - y patterns laid down on glass, allowing a 2-dimensional measurement to be made. However, the γ rejection capability needs to be evaluated, and manufacturing methods to reduce costs also have to be investigated.



Figure 19: Left: The concept of the wavelength shifting fibre readout. Middle: The test setup for the measurements of light loss from bending the fibres. Right: A fibre mounted on the 30 cm \times 30 cm test array currently under construction.



Figure 20: Top left: The principle of the Anger camera. Top right: A prototype of a light guide to reduce the PMT footprint. Bottom: The results of a precision scan of gain of a multi-anode PMT from the test bench for calibrating PMTs. An aspect ratio of 3:1 between the scintillator area and PMT area was chosen for the wavelength guides.





Figure 21: Top left: The concept of a Gd-MSGC detector. Top right: Microstrip plate pattern. Bottom: Digital position resolution from the prototype device, before any algorithms, such as a centre of gravity algorithm is applied.

 BF_3 gas detectors. Historically, BF_3 detectors were superseded by ³He detectors. As such it is of course an option to roll back to the previous generation of technology. However, the performance of BF_3 is not equivalent to ³He under the same conditions – and therefore to compensate for this, higher pressure and/or more layers are needed. As part of the JRA activity, ILL and HZB are looking into BF_3 detectors, with Centronic as an industrial partner, in particular for the safety aspects. Here, in particular, HZB needs BF_3 detectors for the upgrade of the NEAT detector. The present set of prototypes are having problems in matching the expected performance. As such, the complication level can be considered to some extent to be comparable to that for the multi-layer ¹⁰B concept. Overall, the safety issue is the biggest problem, in particular for testing, handling and transport. This results in high costs involved in mitigating these risks. Technical solutions to these problems are being solved in principle by the ongoing JRA collaboration. At the end of the day, however, there is the issue that it is a constant risk. Therefore, mainly for safety considerations, BF_3 is considered only as a backup of last resort.

2.4.2 Choppers

Sophisticated chopper systems are crucial to fully exploit the potential of a long pulse source such as the ESS. Different strategies such as frame rate multiplication [49] try to use as much as possible of the long pulse to benefit the instruments, not only from the increase in peak intensity, but also by accessing a large dynamical range, making the ESS neutron scattering instruments unique. Guide systems with (probably) high cross sections will be used in combination with high frequency choppers (either Fermi or disc choppers) in order to fully benefit from the high peak intensity combined with the long pulse structure. Fast rotating Fermi choppers used in combination with large neutron beam cross-sections will imply heavy choppers (in the order of 40 kg or more), that will require specifically designed non-contact, wear free and ideally maintenance-free bearing systems, that is, usually magnetic bearings. The Research Centre Jülich (FZJ) is planning [48]:

- 1. to mock up a heavy Fermi chopper equipped with magnetic bearings and a non-contact drive system to optimise the start up time and the phase stability at different rotational velocities.
- 2. to mock up a multi-chopper design [50], where small and very fast rotating pencil-like choppers will be positioned closely together to simulate one large Fermi chopper. Such an array, where each "pencil chopper" is equipped with a Fermi package, is not limited by weight but rather by the precise control and phase stability, which will be studied during the development.

The Technical University of München (TUM) is investigating high speed chopper discs for instruments that do not require Fermi choppers but rather can use conventional disc chopper systems. These will extend the capabilities of the chopper disc system developed for the cold time-of-flight spectrometer TOF-TOF at FRM-II [51]. The TUM effort will focus on two aspects:

- 1. Important characteristics of chopper discs such as diameter, the intended rotation speed, and the maximum mass determined by the drive system.
- 2. Long term reliability of chopper systems that are exposed to high radiation fields, which are expected to be significantly larger at the ESS, compared to other neutron facilities.

So far, the chopper discs used for TOF-TOF are manufactured from carbon fibre reinforced composite material and are equipped with magnetic bearings and an active control system. The discs routinely operate at a maximum rotation speed of 22,000 rpm. A design study achieved a maximum rotation speed of 27,500 rpm (until failure of the disc) with the constraints imposed by the TOF-TOF geometry [52]. The limitations of the current design have been identified and further development will in all likelihood result in discs with a diameter of 600 mm that can be operated at approximately 28,000 rpm [53].

While the chopper system is crucial for the overall performance of the neutron scattering instruments, it is also of utmost importance to consider the serviceability, maintainability and accessibility (SMA) of the individual chopper systems in order to minimise the "Lost Time Due To Component Failure" (LTCF). Not all of the ESS neutron scattering instruments will require the most advanced chopper systems, and it is therefore essential to use standardised components – chopper discs, bearing and motor systems, and controls – to fully optimise SMA during routine maintenance, and to minimise LTCF in case of unforeseen problems that will occur during operation. It seems worthwhile to standardise on chopper diameters and control systems. This will allow standard chopper housings to be designed that make SMA easy for the technical staff, and which will minimise downtime. An example of a standard chopper housing used at SNS is shown in Figure 22. More complex chopper systems using counter-rotating discs are commercially available as shown in Figures 23 and 24. The final design parameters will depend on the requirements of the neutron scattering instruments.



Figure 22: Standard chopper housing used at the SNS in Oak Ridge. Left: Chopper mounted on a trolley during maintenance. Right: Chopper installed at the beamline. All critical supplies such as cooling water and electronics are accessible via the top mounting plate. All housings are standard for SNS instruments irrespective of the actual guide dimensions.





Figure 23: Left: Commercially available chopper system. Right: Rack mounted control unit. The control unit can easily and quickly be replaced, thus minimising LTCF in case of unforeseen electronic failure.





ESS itself will be responsible for operation and maintenance once the neutron scattering instruments, built as in-kind contributions to the ESS project, are handed over from the contributing partner laboratories. Risks will be mitigated, and more importantly SMA and LTCF will benefit in the long term, if it is possible to choose external and commercial suppliers. Standardisation of mechanical and electronic systems related to chopper systems, wherever possible, is even more important with regards to the ongoing costs related to keeping standard sets of spare parts instead of individual and instrument-specific hardware solutions.

2.4.3 Neutron optics

The neutronic performance of the neutron scattering instruments will rely not only on the chopper systems described in the previous section, but also on novel and innovative neutron optical systems tailored to the requirements of the individual instruments. The unprecedented peak intensities will enable the ESS to investigate samples with volumes of the order of mm³ rather than cm³, and will make neutron optics the key technology to deliver highly intense neutron beams onto small sample areas.

Several sub-projects have been defined in order to explore different focusing options [55]. The main issue of investigating small volumes is focusing neutrons, which is primarily done by focusing neutron guides, that is, by systems based on supermirror technology [56] that use large m values to reduce the cross section of a guide with typical dimensions of 15 cm × 5 cm down to 3 cm × 3 cm (height × width). The use of more sophisticated shapes, such as elliptical or parabolic guides, are intended to increase the intensity over a small area. Measurements on prototypes of parabolic and elliptic focusing guides using supermirror coatings m = 3 have demonstrated that it is possible to achieve considerable flux gains on spot sizes of the order of 1 mm² [57, 58]. The practical use of focusing guide elements at regular neutron beamlines revealed the following problems:

- difficulty of aligning the focal point on tiny samples,
- adaptation of the beam size to the sample size and position, and
- optimisation of the divergence of the neutron beam with respect to the sample



Figure 25: Left: Design of prototype II adaptive optics, including five micro-linear stages for flexibly adjusting the supermirror substrate to a parabolic shape. Right: The first realised device.





Figure 26: Measurement with prototype II, showing a gain in intensity of about a factor of 6.

Adaptive optics. Several adaptive focusing devices are currently being tested at the PSI, to resolve these problems [55]. One way to adjust the focusing characteristics of a neutron guide is to change the curvature of the focusing device. Figures 25 and 26 show how the concept of bending a uniform substrate by 5 actuators is achieved in one of three different concepts that have already been investigated and measured at the BOA beamline at SINQ (PSI). Adaptive focusing can also be achieved by using the recently introduced Compound Refractive Lenses (CRL) [59], or by using Fresnel lenses [60].

Compound refractive lenses. A CRL microscope has been used recently to produce magnified images of materials containing hydrogen, for which the main contrast mechanism in case of neutrons is incoherent scattering. Here, the CRL was composed of 100 MgF₂ biconcave lenses that produced magnified (\times 22.5) images of polyethylene and polypropylene (hydrogen rich) grids and biological specimens using 8.5 Å cold neutrons with a 10% bandwidth, as shown in Figure 27 [61]. New CRL-based neutron optics will be explored to improve their performance and minimise optical errors. Several focusing devices, aimed at focusing neutron beams onto small samples are currently being tested at PSI [55], and analytical calculations as well as Monte Carlo simulations will accompany the optimisation of novel neutron optical components.



Figure 27: Left: A scorpion and a leaf. Right: Neutron image of scorpion made from two stitched partial scorpion images at 10.0 Å and 300 seconds [60].

Crystal Optics. Mosaic [62] and bent perfect crystals [63] for monochromating and energy-analysing the neutron beam are in standard use at steady-state sources. The high time-average brightness of the ESS would allow these methods to be used at a pulsed source, with the source time structure being used, for example, to separate higher orders. Multiplexed monochromator and analyser systems which select several wavelengths simultaneously will be studied to make effective use of the ESS time structure. Development of new crystals, such as diamond for short wavelengths [64] or GaAs [65] for very high resolution applications, could open up significant new possibilities.

Polarisation. Polarising supermirrors based on various multilayer systems, such as Fe/Si and FeCoV/TiNx, are used in neutron instrumentation to provide a polarised neutron beam and to analyse the polarisation of the scattered beam. The multiple magnetic and nonmagnetic layers have different scattering contrasts for neutrons with either up or down polarisation. Moreover, the internal stresses of the multilayer systems are manipulated in such a way that the polariser can be used in its remanent state. In particular, FeCoV polarisers have the property that the magnetisation can be induced with an external magnetic field of only 2–4 mT. This feature makes the FeCoV polariser very important if polarisation is needed together with a cryomagnetic sample environment. The further development of polarisers will be realised at PSI. The 60 degree supermirror analyser based on FeCoV/TiNx multilayers that is shown in Figure 28 was built and tested at SINQ/PSI in 2011. It reached a polarisation of more than 95% with a transmission of 45% for the spin up component at 5 Å. The main feature of the device is that the assembled 960 polarisers are positioned without any gaps. The present limitation of the FeCoV polariser is the maximal m value of around 3. The goal of the project is to increase the quality of the polariser – a higher m value without a significant decrease in reflectivity – and to reduce the potential for ⁶⁰Co activation.

³He devices. Long pulses require polarising devices to be effective over a broad wavelength band, and to be able to cope with an increased angular acceptance. Conceptual designs of an in-beam Spin Exchange Optical


Figure 28: Left: Reflectivity curves (spin up and down) for a FeCoV polariser. Right: Wide angle analyser (60 degrees) without gaps based on FeCoV/TiNx polarisers.

Pumping (SEOP) analyser that can be used for a small angle neutron scattering instrument, which does not use supermirror technology, are currently being investigated [48]. Software has been developed that allows precise magnetic field calculations for complicated systems of permanent magnets, coils and magnetic screens. This enables a long magnetic life time for ³He in the cell, and consequently high polarisation.

2.4.4 Sample environment

Sample environment plays a key role for the success of a neutron user facility – the variation of parameters like temperature, magnetic or electric field, pressure, humidity or gas flow is in almost all cases an essential part of a neutron experiment. These sample parameters have to be provided in a very reliable way and in a broad range. Temperatures from mK to thousands of degrees C, magnetic fields from "zero" to 17 T, and pressures up to several GPa are standard at contemporary leading neutron sources. The high flux ESS will have special requirements in regard to its sample environment devices, beyond simply providing broad access to parameter space. Waiting times – for example, for temperature equilibration or for sample changes – have to be minimised for optimal beam time usage. New experiments, formerly not possible, will need new kinds of sample environment.

A modular approach is promising, with interchangeable sample environments for standard experiments, combined with highly specialised sample environments for highly specialised neutron experiments. Standardisation of mechanical dimensions and software interfaces will help to ease the fast exchange of sample environment devices. Controls and cabling can reach a high level of complexity. The standardisation of procedures and systems has been the best practice in leading institutions worldwide, minimising potential errors and the loss of precious beam time [48].

Consultation with the different local user communities and with leading researchers is of paramount importance in determining the top priorities and future research trends. The present necessities for instruments need to be addressed, and future trends need to be anticipated, allowing critical scientific experiments to be performed in a timely manner. An instrument-specific sample environment that will probably operate synchronously with the ESS pulse structure will be developed in more detail, once a firm decision on the 7 day one instruments has been reached. Nonetheless, it is reasonable to anticipate that the sample environment could include:

Low temperature and magnetic fields.

- Superconducting (asymmetric) vertical and horizontal cryomagnets.
- Modular low temperature inserts (dilution and ³He).
- Pulsed high field magnets (≥ 40 T) with ultra-fast repetition rates.
- Cryogenic polarisers that allow access to magnetisation distributions in molecular magnets, nanoscale samples, et cetera, on powder diffractometers.

• Magnets with arbitrary angles with regard to the scattering vector, that are useful for investigating complex magnetic structures including multiferroics.

High temperature and pressure.

- Vacuum furnaces and *in situ* reaction chambers. Levitation furnaces that are part of the European NMI3 project will greatly improve the ability to assess materials at higher temperatures and will have an important impact on research about high temperature innovative materials.
- Dedicated and optimised pressure cells that, for example, reproduce conditions found deep within the earths crust that are of interest to the geophysical community, but which could also address other scientific problems and needs.

Soft matter. A priority list of equipment for the soft condensed matter group will be developed together with the user community. Some developments are likely to include:

- Shear cells where the shear direction is perpendicular and/or parallel to the neutron beam direction.
- Sample cells for fast and accurately controlled temperature and pressure jumps.
- In situ liquid handling on ml and μ l volume scales [55]. This will also be developed for neutron reflectometers.
- Stopped flow devices for SANS and surface studies.
- Kinetic experiments with variable external parameters such as temperature, humidity controlled environments, controlled gas environments.
- Sample environments for complementary *in situ* and *ex situ* techniques, such as light scattering, UV-Vis and infrared spectroscopy, ellipsometry, X-ray reflectivity and diffraction, and AFM.



Figure 29: Contemporary sample environments that require modification for use on the ESS neutron scattering instruments. Left: Shear cell. Right: Variable angle spectroscopic ellipsometer.

Some existing equipment – such as that shown in Figure 29 – is already available commercially or is already developed, but requires modification for use on the ESS neutron scattering instruments. Other hardware needs development, taking of the order of up to four years. Development should not start too early in order to ensure that:

- one can benefit from further commercial development
- specific environments do not become obsolete by the time that the first seven instruments become operational.

Material science. Materials scientists not only need furnaces for the application of high temperatures, but also (for example) need load frames for the application of external forces, and a combination of both. Such devices must rotate in the neutron beam, for example for texture measurements. A 6-axis robot arm, similar to the one shown in Figure 30, will help texture and other measurements, and will help to achieve a high sample throughput and short data acquisition times. However, robotic systems are not only limited to applications in material science but are also useful, for example, for soft matter applications with high throughput.



Figure 30: The robotic system for automatic sample manipulation installed at the materials science diffractometer STRES-SPEC at FRM-II [66].

Electronics and hardware control. Major issues that need to be addressed include data acquisition systems, motion control, safety interlock systems, and general automation with an emphasis on standardisation, maintainability, and compatibility between instruments and instrument control systems [67]. This interfaces with the responsibilities of the DMSC, which is responsible for programming and computing efforts related to the neutron scattering instruments such as instrument control, data reduction and data analysis.

In terms of risk mitigation and in order to benefit from innovations in the ESS Accelerator and Target Divisions, it is attractive to consider the Experimental Physics and Industrial Control System (EPICS) that will be used by both divisions. EPICS [68] is a software environment used to develop and implement distributed control systems to operate devices such as accelerators, telescopes and other large experiments. EPICS also provides SCADA – Supervisory Control and Data Acquisition Capabilities – for systems that feature large numbers of networked computers providing control and feedback. EPICS interfaces to the real world via Input Output Controllers (IOCs) that are standard PCs or VME, PCI, ATCA, et cetera. IOCs are standard embedded system processors that manage a variety of "plug and play" modules (GPIB, RS-232, IP Carrier et cetera) that interface to control system instruments (oscilloscopes, network analysers) and devices (motors, thermocouples, switches, et cetera). Many relevant drivers already exist, such as for:

- Galil Ethernet DMC-22x0 and DMC-40x0 standalone multi-axis motion controllers,
- Cryojet controllers, Cryojet Autofill controllers from Oxford Scientific,
- Lakeshore temperature controller and Pfeiffer Vacuum systems

One of the main advantages of EPICS is that it is a quasi-industry standard, so it is well maintained and documented, and has the support of a large number of large scale facilities, such as the Australian Synchrotron, Diamond light source, Swiss Light Source, Los Alamos Neutron Science Center, and the Spallation Neutron Source. The SNS is gradually upgrading their EPICS systems to unify the existing accelerator and target control system with the neutron scattering instruments. Standardising early in the project will benefit the ESS in the long term with respect to SMA and LTCF, and will reduce running costs. The electronics group in the

Science Division will require less overhead due to synergies with the Accelerator and Target Divisions. Potential development for the ESS instrument specific EPICS drivers can be done in close collaboration with the SNS as well as with personnel in the Integrated Controls Systems group. This will free valuable resources that can more effectively be used to develop the ESS specific event mode data acquisition system, as described in section 6.1, in close interaction with the ESS collaboration partners such as PSI. Most of this effort is expected to take place between 2012 and 2014.

2.5 Potential upgradeability

The current design report is necessarily focused on delivering the hardware and science capabilities within the scope of the project. It is, however, important to bear in mind what the future upgrade paths might be, so as not to unnecessarily exclude or compromise future possibilities should they come available.

Number of beamports. The preferred upgrade path to increasing the number of instruments beyond the currently envisaged 22 is to increase the number of beam ports on the main target station, rather than to build a second target station. Current design efforts indicate that it may be possible allow for significantly more than 40 beam ports, which in the long run would be a far more economical way of increasing the scientific output of the ESS than building a second target station. It would also represent a more efficient use of the accelerator and the neutrons produced. Building a second target station, even if one ignores the very high cost of such an option, would require an increase in the accelerator power in order to feed both target stations, just to maintain the brightness of the first target station. With a single target station, any increases in accelerator power would result in increased neutron brightness for all instruments. The reduced beam separation imposed by designing in a larger number of beam ports, places constraints on the design of the shutters and the choppers and other beam-shaping equipment both within and close to the target station monolith, which are currently being studied.

Hot neutrons. The source brightness of neutrons with wavelengths below about 0.6 Å will not be significantly higher at the ESS than at the present high flux sources. Particularly in the epithermal neutron range, high power short pulse spallation sources will most likely outperform a long pulse source for high resolution applications. If a hot source were to be installed at the ESS, the instruments that it would serve would probably not be able to make efficient use of the source time structure, which is better suited to thermal and cold neutrons. Such instruments would therefore operate in a similar manner to hot source instruments at steady state sources. In order to maintain a healthy community and an ever-increasing scientific output of high quality research with neutrons in Europe, it is essential that the European neutron landscape consists of a network of several medium to high flux sources and is not just concentrated on one high end source like the ESS. The ESS management will work actively together with other neutron centres to maintain such a healthy neutron landscape in the future. If the future neutron landscape includes neutron sources with good performance for hot neutron instruments, the ESS would not have to cover this area.

High reliability mode. The current baseline of 95% reliability represents a considerable improvement over existing pulsed sources. However, for some parametric and real-time measurements, reliabilities of the order of 98%–99% are needed. These experiments are currently restricted to reactor-based sources with their intrinsically high reliability. A study needs to be undertaken in how to increase beam availability at the expense, perhaps, of time averaged neutron flux. Preliminary analysis indicates that reducing the pulse length would have the most direct influence on accelerator reliability – more so than reducing the peak current or the repetition rate. A more complete and quantitative study will be undertaken to study how a high reliability mode might operate and at which potential cost to the flux on the instruments. A certain fraction of the beam time of the ESS might then be offered in this high reliability mode.

3 Target Station

3.1 Principles and design choices

The target station shown conceptually in Figure 31 performs 3 key functions in a spallation neutron source. It:

- a) transforms the proton beam radiation impinging on the heavy metal target into fast neutrons as the desired product, and a large amount of radioactive isotopes and radiation as largely undesirable by-products,
- **b)** transforms the fast neutrons emitted by the target into slow neutrons via moderators and reflectors, which are the final form of radiation provided by the source, while further radioactive by-products are produced by the absorption of these neutrons by various facility components, and
- c) provides intense slow neutron beams through beam ports accessible at the exit of the target shielding for delivery and use at the neutron scattering instruments around the target, fed by these beam ports.

In this context "fast" means neutrons that travel at about 10% of the speed of light, while "slow" neutrons move at about the speed of sound. The main requirement for a target station is for it to perform these key functions efficiently, safely, and in full compliance with legal safety standards and requirements for:

- 1. the release of radioactivity and disposal of radioactive waste in normal operation,
- 2. controlling and mitigating the consequences of operational accidents, and
- 3. robustness in the case of external influence of natural or manmade disasters (earthquake, airplane crash, et cetera)

The target station consists of:

- 1. the target itself that performs function **a**),
- 2. a neutron moderator, pre-moderator and reflector system that performs function b), and
- 3. a beam extraction system for function c).



Figure 31: General conceptual layout of the target station. The target monolith is shown at the left, with representative neutron beamlines on the right.

Furthermore, the target station incorporates powerful cooling systems in order to be able to absorb the 5 MW proton beam power. It contains about 8,000 tons of shielding material inside the 12 m diameter of the target monolith in order to reduce to acceptable safe levels the ionising radiation escaping from the target station outside the slow neutron beam ports.

Safe cooling. The main underlying technical design challenge of the target station design is the provision of efficient and safe cooling for the energy deposited by the proton beam with very high peak heating density in the range of 3 kW/cm³. This challenge has two aspects: to circulate large amounts of coolants while also assuring safety in the case of coolant system failure – both on-site for the workers and off-site in the urban environment. The coolant stream is in the range of 3 kg/s for helium gas, 15 kg/s for water, and 300 kg/s for liquid metal cooling. The most critical design responsibility is assuring safety at this power level, which is unprecedented for a spallation neutron source, or for any other accelerator based facility.

The most probable operational reason for a cooling system loss is an electric power interruption in the grid. Although this guarantees an instantaneous shut-down of the accelerator, heat production in the target will continue on a gradually decreasing but significant level for months, because the target accumulates a considerable amount of energy during operation in the form of radioactivity, part of which is released as heat over an extended period of time. Without cooling this after-heat increases the temperature of the target. The risks represented by this phenomenon are reduced to zero by adopting a design that guarantees sufficient passive cooling by heat exchange with the environment, so that the maximum temperatures remain safe everywhere in the target station, even in the operational absence of any active cooling system. A more costly solution – that is not fully free of residual risk – is to build and operate a failsafe emergency electric power system that keeps the cooling system in operation during grid power cuts. For the case of cooling failures not related to a general electric power cut, failsafe interlock systems are required to shut-down the accelerator beam production within a fraction of a second.

Target. Target station performance – in terms of both neutron yield and safety – critically depends on the choice of the target material, and on the provision of adequate cooling. The ESS has selected a rotating tungsten wheel as the baseline option for the target, with a metallic liquid lead bismuth eutectic (LBE) solution as a comparative option. (Two alternatives are necessary in order to present a broader picture on environmental impact to the licensing authorities.) Both options offer comparable neutron yield performance, and satisfy the safety goals for waste disposal in normal operation. Both of these technologies are new for spallation sources; none of the well-established target design solutions is adequate for the higher power level of the ESS. In case of an unexpected problem with the realisation of the baseline option, a fall-back solution will be selected on the basis of the accumulated state-of-knowledge at that time.

In the case of loss of active cooling, a rotating, helium-gas-cooled tungsten target of 2.5 m diameter safely offers a large enough surface for passive radiative cooling, avoiding dangerous temperature excursions with a significant safety margin. By contrast, this might not apply to a water-cooled tungsten target of the same dimensions using established corrosion protection technique, for two substantial reasons. Firstly, the tantalum cladding necessary to protect the tungsten from the highly corrosive cooling water adds considerably to the after-heat. Secondly, both tungsten and tantalum enter into a vigorous exothermic chemical reaction with water vapour above about 700 C. This is much lower than the safe limit of 900 C that applies for a helium gas cooled target wheel, corresponding to about 820 C for the steel target envelope. The equivalent liquid metal target can be made safe with passive cooling by choosing a large enough volume – more than about 1 m³ – of LBE circulating through a large enough reservoir tank. The after-heat production is then uniformly distributed in the liquid metal volume.

Helium gas cooling is therefore chosen for the baseline rotating tungsten target (see section 3.2). Water cooling represents a potential alternative, although prior experience is available only at relatively low spallation power levels (see section 3.1.1).

Moderator, pre-moderator, and reflector. The target station contains two liquid hydrogen moderators of about a litre volume each, partially surrounded by water pre-moderators of comparable volume. The moderators are placed inside an inner reflector of about 1 m^3 of beryllium. These components will be kept at their desired operational temperature by dedicated cooling systems that remove the heat deposited by the high level of radiation during operation. These systems will not emit significant after-heat.

Beam extraction. The beam extraction system consists of a number of beam tubes arranged in 4 sectors of $60 - 65^{\circ}$ angular spread in the horizontal plane. Adequate free space around the neutron emitting moderator surfaces ensures an unobstructed view of these surfaces by all beamlines in each sector. The dimensions of the beam tubes across the target shielding is sufficient to accommodate advanced, complex neutron guides. Each beam tube is equipped with a beam shutter within the target monolith, ensuring that the residual radiation escaping through the closed beamline is reduced to levels offering a safe working environment outside the target monolith, for unlimited periods of time when the target station is not in operation. The target monolith is surrounded by a combination of integrated and individual radiation shielding for each beamline, guaranteeing

safe working access to the areas outside of these shielding structures all the time, including during full power operation.

The target monolith provides two barrier layers of containment against the escape of volatile and airborne radioactive materials, both during normal operation and also in case of incidents. The contained volumes are continuously vented and filtered. The unavoidable residual escape of radioactive effluents in amounts below the limits authorised in the operational license is channelled through a controlled release stack, after collecting these gases from all over the facility.

Components exposed to the proton beam, and/or to the high radiation environment around the target, have a limited lifetime ranging from a few months to several years – short compared to the several decades of ESS operations. These components become highly radioactive. Their periodic replacement, handling, and storage before disposal, is accomplished with the help of remote control and adequate protective equipment, including hot cells and casks at various locations around the target monolith. Equipment parts that are regularly replaced are organised in modules, for safe and simplified handling. They consist of the accelerator beam window, the target (together with its supporting structure and containment shroud), and the moderators (together with their pre-moderators and the inner reflector).

These replacements offer the important opportunity to improve the design of components central for the neutron beam production efficiency. The modular approach to the renewal maintenance procedure enables future new developments that will enhance ESS performance. Specific consideration is being given to developing remote robotic maintenance and operation methodologies for increased effectiveness and reliability and reduced radiation doses to individuals. This primarily concerns the pre-moderator, moderator, and reflector systems, where continual progress is expected through new materials and improved lay-outs. Together with the inherent potential of power upgrades, this upgrade potential allows a cost-effective way for the ESS to remain the premier state-of-the-art spallation neutron source for a half a century.

3.1.1 Water cooling options

Tungsten has often been chosen as target material at spallation sources, because of its high neutron yield related to its high density. Extensive experience with water cooled tungsten targets is available, gained over some 4 decades, for beam powers up to about 250 kW with stationary target configurations in which all the proton beam power is deposited into about 2 litre of target material. This represents a huge body of knowledge from which a design of a water cooled target design could be developed; many of the problems are known and solutions have been found and tested. However, ESS represents a 20-fold leap in power (and in neutronic performance), calling for new technologies. The rotating target approach is based on the main consideration that the target lifetime is maintained at a reasonable value by increasing the irradiated target volume in proportion to the power increase, since the total radiation damage to the tungsten target material and to its envelope will be kept at the same level as in existing spallation sources, such as ISIS or the Lujan Center. This also applies to the time average heat deposition density in the target volume – that is, the cooling needs are designed for the same performance in terms of heat removal per unit volume, while the total heat removal is increased in proportion to the total beam power.

Closer examination shows, however, that several key issues in cooling the target do not simply scale with the time average proton beam energy deposition density. These result in fundamental changes in both the technical parameters and in the safety requirements, which imply considerable R&D efforts for the development of water cooling technology for spallation targets at the 5 MW power level. In the following the main issues are described together with foreseen implications on the design and possible ways around them.

The extension of the target volume in proportion of the power increase cannot be reasonably accomplished by maintaining the surface to volume ratio of the existing solid spallation targets: even for a large, 2.5 m diameter rotating target wheel the footprint surface area per MW of beam power is less than half of (for example) ISIS. This means that in the case of loss of cooling during stopped beam operation (for example during an electrical power cut) the after-heat will raise the target material to higher temperatures. With increasing temperature in the presence of water vapour, the exothermic water reduction process of the type much studied for Zircaloy in the nuclear industry,

$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2$$

causes the tungsten target material and also any tantalum cladding material to vaporise into airborne oxides. The simultaneously produced hydrogen gas can accumulate and produce additional heat and/or damage by catching fire. This reaction and the associated risks need to be very carefully analysed and mitigated, and the results need to be presented to the licensing authorities.

The critical temperature for tungsten in the presence of water vapour is estimated to be 700 - 750 C, above which the release of airborne radioactivity is qualified as a radiological accident effecting people outside the

borders of the facility. Water vapour is unavoidable in the case of loss of cooling efficiency with a water cooled target even if the proton beam is shut-down: the 60 kW initial radioactive decay after-heat emitted by tungsten and the tantalum cladding (see below) can evaporate about 1 litre of cooling water every minute. The target will reach a temperature within 100 - 150 C of the critical temperature (assuming surface treatment for high heat radiation emissivity, such as sandblasting), under the effect of the after-heat without active cooling for a target at 5 MW proton beam power. This does not leave enough headroom for a convincing margin for the safety case, and it excludes all possibility of a future power upgrade. In conclusion, the use of water cooling for the rotating tungsten target requires envisaging an emergency cooling system for ESS, such as the redundant, fail-safe back-up power generation systems used at nuclear power plants. Such an elaborate cooling safety approach can certainly be implemented, but it is foreseen to require substantial additional resources and will make the licensing process more demanding. (Gravity driven emergency cooling systems have been proposed in the nuclear industry, but they are not licensed in Sweden.)

An alternative approach is to modify the target design, choosing other materials so that the after-heat and its effects are reduced while the neutron production level is kept high. Since a large fraction of the after-heat is generated in the tantalum cladding, one way would be to develop a new cladding or canning technique for tungsten with a material less sensitive to water vapour, that generates less after-heat. This is however a substantial and long term R&D effort. A particular challenge with cladding is the swelling of irradiated tungsten above 600 K, and with the need to provide sufficient thermal contact between the tungsten target material and the can. Similarly, tungsten could be exchanged for a material less efficient in producing neutrons, generating less after-heat and less sensitive to water vapour. This would, however, clearly impair the neutronic performance and would also require a substantial R&D effort.

In other types of accident the source of heat is not only the after-heat generation. These include fire and the failure to automatically switch off the proton beam when the target cooling is out of order. For example, if the target rotation stops and the beam is not switched off before the next proton beam pulse, then cooling water evaporation will start in the target wheel at an equivalent rate of 200 litres of water vapour per second at 10 bar and at 180 C, while the temperature of the target itself increases at a rate of 1500 C per second at its hottest spot. Such scenarios also require measures to be taken to avoid exceeding the critical target temperature when water cooling is used (and to mitigate the consequences, if these measures fail).

Thus water cooling impairment accidents at ESS power levels result in a very complex safety situation within the fraction of a second, further aggravated by the onset of exothermic hydrogen gas production well before 1 s. The analysis and the mitigation of the consequences of such an accidental scenario requires extensive studies, most of it on fully uncharted territory in view of the unprecedented power deposition density of the ESS accelerator beam. Qualifying these types of accidents as "beyond baseline" will require proving that the proton beam shut-down systems will fail with a probability of less than once per 1 million years, or it will require the implementation of a hard wired back-up, passively failsafe beam shut-down system with a proven very fast response time. In the case of water cooling this response time must be in the range of one second. The inertia of the wheel and the cooling water might make the technical circumstances and the demands on the cooling and safety systems less severe than than these initial indications.

Another main aspect of water cooling that does not scale with the time average heat deposition density is the temperature jump in the target during a single proton beam pulse. At 5 MW power this will exceed 100 C at the hottest part of the target. Including a safety margin leads to the need to consider 200 C. (In contrast, this temperature jump is just a few degrees C at the power level of existing spallation sources.) This will substantially enhance the risk of the onset of film boiling at the boundary between coolant and target. Mitigation might require using elevated water pressures in the target wheel, eventually adopting the boiling water cooling method well established in the nuclear industry. Pulsed heat deposition from the proton beam directly into the water also produces a pressure wave in the coolant, another new phenomenon that has not been explored in the existing spallation environments.

The presence of water inside the target adds to the radioactive inventory of the facility in two ways: water gets directly activated by the proton beam and the neutrons, and the neutron moderating effect of water within the target enhances the activation of the target tungsten. The presence of hydrogen atoms in the light water coolant is known to reduce the neutron flux compared to heavy water. Using heavy water as coolant, on the other hand, enhances tritium production and release, and adds substantially to the operational costs and complexities.

The radiation environment enhances the corrosive power of water. Tungsten is known to be insufficiently resistant to water under spallation conditions and there is extensive experience with using tantalum cladding as corrosion protection for tungsten. Tantalum cladding, however, also enhances some risks: its after-heat after irradiation is higher than that of tungsten, thus it reduces the safety margin for passive cooling of the target in case of electric power loss. It also interacts with water vapour at elevated temperatures, and tantalum cladding is known to easily develop cracks. Above 600 C irradiated tungsten swells in the range of 1-2% in volume,

which is possibly detrimental to the tantalum cladding.

Leaks of water coolant are frequent in the spallation environment and remediation measures are widely used and tested. New issues need to be addressed in this respect too, at the 5 MW power level. The rotating target principle, without which water cooling would not be feasible at all, enhances the risks of leaks and spills by the necessity of working with rotating seals for the coolant. In the environment of radiation containment barriers, which include the target building itself, the risk of spilling water at temperatures above 60 C adds to the pressure resistance requirements towards the building, which has a significant impact on costs.

3.2 Helium cooled rotating target system

The RoTating Helium-cooled Target (RoTHeTa) concept is based on a rotating tungsten wheel. General target parameters are summarised in Table 7, while high level ESS parameters are shown in Table 2. Figure 32 illustrates the general layout of the rotating wheel. Helium is continuously blown through the target, which is composed of angular sectors, or *slices*. Each slice is composed of annular tungsten plates of different thickness, as shown at the bottom of Figure 32. The number of slices depends on the beam width and the wheel diameter; it also dictates the revolution rate. The target material is internally supported by the *target shroud* structure. The spallation material and the cooling fluid enclosed in this shroud are divided in 3 parts: the top and bottom shroud plates and the *beam entrance window*. The radial length of spallation material is long enough to stop all primary protons, avoiding the need to have an active beam dump.

Parameter	Unit	Value
Outer diameter of the wheel	m	2.5
Revolution rate	rpm	25.45
Number of angular sectors, or slices		33
Helium pressure inside the wheel	bar	3.0
Shroud thickness (steel)	mm	4.0
Beam distribution		Parabolic
Beam footprint width	$\mathbf{m}\mathbf{m}$	160
Beam footprint height	mm	60
Power removal (60% of proton beam power)	MW	3.0
Helium inlet pressure	bar	3.0 - 3.5
Helium outlet pressure	bar	2.5 - 3.0
Helium mass flow rate	$\rm kg/s$	3
Helium specific heat	J/(kg.K)	5193
Helium temperature rise, ΔT	Κ	200
Helium loop volume	m^3	2 - 15

Table 7: General parameters of the rotating target system.

3.2.1 Target holder

Shroud. A study of the mechanical stability of the shroud has been performed, allowing 3 parameters to vary: (i) the helium pressure inside the wheel, (ii) the thickness of the steel shroud, and (iii) the sectorisation angle between slices. The rotation of the wheel and the effects of gravity were taken into account, but thermal effects have not yet been incorporated. It was found that using helium pressures larger than about 10 bar would be challenging, but that a shroud thickness of 4 mm is reasonable with a pressure of about 3 bar.

Bearings. A long shaft handling option has been chosen, allowing the drive and rotating components to be outside the region of high neutron flux [69]. Thus, requirements for bearings are relaxed. A simple mechanical solution is adopted, using experience-proven mechanical ball bearings that are lubricated with graphite rather than grease, to reduce activation even further, even though irradiation-qualified bearings will be used.

3.2.2 Cooling performance

Helium moves radially out between two slices, and then flows azimuthally between the plates, before flowing back towards the shaft through the radial channels between the two neighbouring slices. This helium flow also cools the beam entrance window. The helium inlet pressure listed is the minimum necessary for the overall cooling loop. The global helium temperature increase ΔT (between entering and exiting the target) is limited by the temperature allowed in the hot part of the helium loop. This then sets the minimum helium mass flow rate. The helium cooling loop parameters shown in Table 7 could be revised, according to the exact material choice and its creep behaviour. Figure 33 shows preliminary estimations of helium cooling performance in the wheel, demonstrating the practical feasibility of the system.



Figure 32: Sketches of the target wheel. Top: Radial and azimuthal flow of helium around the slices. Bottom: Global geometry, showing the angular sectorisation into slices.



Figure 33: Temperature (top), velocity (middle), and pressure (bottom) distributions from simulations of a RoTHeTa system. The thickness of the tungsten target slabs increases as the heat deposition density decreases along the proton beam direction. The operational parameters (for example target temperature profile, top) can be tuned by the choice of these thicknesses. In the example shown the thinnest target slab is 13 mm thick.

Location	Pressure drop [bar]	Comment
Across the target	0.30	Calculated
In the shaft and straight pipe	0.05	Calculated
Inlet rotating seal and feedthrough	0.10	Specified
Outlet rotating seal and feedthrough	0.10	Specified
Filtering system	0.12	Calculated
Heat exchanger	0.30	Calculated
Rest of loop	0.03	Specified
TOTAL	1.00	

Table 8: Pressure drop summary in the helium cooling loop.

Parameter	Unit	Value
Helium mass flow rate	$\rm kg/s$	0.012 - 0.12
Helium pressure	\mathbf{bar}	3 - 6
Temperature	\mathbf{C}	20 - 250

Table 9: HELOKA-LP helium loop characteristics, at KIT, Karlsruhe.

Parameter	Unit	Value
Inlet pressure	bar	3.0
Outlet pressure	bar	4.0
Number of stages		4
Shaft power	kW	807
Shaft rotation speed	rpm	11,710
Outlet temperature	Κ	350
Pump system width	m	7.6
Pump system length	m	3.7

Table 10: Helium loop pump system parameters.

3.2.3 Helium loop

Figure 34 presents the nominal layout of the helium cooling loop. Table 8 summarises the pressure drops that are foreseen in the different parts of the loop. The low pressure and high mass flow loop is similar to the HELOKA-LP loop at KIT, where the maximum mass flow rate listed in Table 9 is lower than for the whole ESS loop. Nonetheless HELOKA-LP, as shown in Figure 35, is sufficient to test a portion – a slice – of the RoTHeTa concept.

Helium compressor. A multistage helium compressor similar to the ROOTS Dresser device shown in Figure 36 is well suited to be the helium cooling loop pump. Figure 37 shows the performance characteristics of such a compressor, with parameters listed in Table 10.

Heat exchanger. The gas-gas (helium-nitrogen) heat exchanger eliminates the potential for water to leak into the helium loop, and thereby to get in contact with the hot tungsten. Table 11 summarises the main parameters of this system.

Parameter	Unit	Value
Heat exchange power limit	MW	3.02
Material		SS 316L
Weight (empty)	kg	$3,\!673$
PRIMARY LOOP		
Fluid		Helium
Mass flow rate	$\rm kg/s$	3.0
Fluid speed	m/s	92.7
Design temperature	Ċ	240
Temperature, inlet	\mathbf{C}	212.5
Temperature, outlet	\mathbf{C}	19.85
Design pressure	\mathbf{bar}	6
Absolute pressure, inlet	bar	3.00
Absolute pressure, outlet	bar	2.77
SECONDARY LOOP		
Fluid		Nitrogen
Mass flow rate	$\rm kg/s$	71.5
Fluid speed	m/s	62.5
Design temperature	Ċ	80
Temperature, inlet	\mathbf{C}	0
Temperature, outlet	\mathbf{C}	40
Design pressure	\mathbf{bar}	12
Absolute pressure, inlet	bar	10.0
Absolute pressure, outlet	bar	9.5

Table 11: Heat exchanger system parameters.

Parameter	Unit	Value
Particulate concentration at the inlet Expected emissions	$ m mg/m^3$ $ m mg/Nm^3$	$0.308 \\ 0.00001$
Expected separation efficiency	%	99.99988

Table 12: Cyclone filter system parameters.

Dust filtering system. Erosion of the tungsten target in the helium gas stream might eventually lead to tungsten dust production. Standard filters are appropriate for smaller particles while the use of cyclone filter systems is highly efficient for filtering larger particles in the gas stream. Cyclone filters like the one shown in Figure 38 are widely used in industry, even in harsh environments. Figure 39 illustrates the filtering efficiency of cyclonic filters as a function of dust particle size, while Tables 7, 8 and 12 list the parameters of the system.



Figure 34: Target helium loop flow diagram.



Figure 35: The HELOKA-LP helium loop at KIT, Karlsruhe.



Figure 36: The ROOTS Dresser multistage helium compressor pump.



Figure 37: Multistage compressor map characteristics, calculated for Roots HN-194 with variable speed.



Figure 38: Cyclonic filtering, in the geometry of the Hurricane PH-150 from ACS.



Figure 39: The predicted grade and global efficiency for a typical cyclone filter system, showing high efficiency for particles larger than about 1 μ m.

3.3 Neutronic performance of the target-moderator-reflector system

The goal of the ESS accelerator and target facility is to produce intense beams of thermal and cold neutrons to the users. The target-moderator-reflector (TMR) system must be optimised in order to provide the highest possible source brightness. The optimisation is done in the neutronic design, by means of Monte Carlo calculations using particle transport codes such as MCNPX and PHITS. In Figure 40 the cold neutron flux (integral flux with E < 5 meV), calculated using PHITS is shown. The red colour corresponds to the peak of the cold neutron flux following the moderation process in the liquid para-hydrogen moderator.

The neutronic calculations performed so far have led to a first set of geometrical parameters of the TMR system, although optimisation work is still in progress. Below we discuss a few key parameters, and the sensitivity of the key figures of merits, such as neutron brightness and heat deposition, on the variation of these parameters.



Figure 40: Map of cold neutrons in the TMR system, calculated using PHITS.

3.3.1 Target design

The neutronic design of the target consists in identifying the best geometrical configuration of the TMR system that provides the highest neutron yield. The neutronic design must address important questions like the optimal target thickness, the best beam profile, the amount of spallation material needed, and the sensitivity to engineering parameters (such as type and thickness of materials, and distance between the different components) of the neutron flux.

Beam profile and dimensions. Optimal neutron production is a function, among others, of the amount of spallation material and of the shape of the beam impinging on the target. Tungsten is a very dense material, which offers, compared to other targets, the advantage of a localised neutron production. This advantage comes at the cost of higher power density, and therefore it is important to consider the correct profile of the beam on target. Target thickness and beam profile are two of the parameters that influence the neutron yield, and they have been studied by means of a detailed optimisation program.

Our studies show that, for a parabolic profile, the beam width can be almost as large as the target width, without significant loss in neutronic performance. This is an important result since it will make the cooling of the target easier. In Figure 41 the combinations of the proton beam height and tungsten wheel height leading to given neutron leakage current are shown, for a bare target without a neighbouring moderator or reflector. The results for a full TMR system will be different – this is an illustrative example. In this particular case it is apparent that the peak current (98% or higher) can be reached with a proton beam height from 0 (pencil beam)



Figure 41: Possible combinations of wheel height and proton beam height, keeping the neutron current within the given fraction of its maximal value (obtained with a pencil beam), for a bare tungsten target (without structure around).



Figure 42: Cold neutron flux (E < 5meV) and heat deposition inside the moderator as a function of the distance (in cm) to the target surface.

to about 7 cm. This gives some freedom for the choice of the best beam profile, keeping in mind important constraints such as peak energy deposition in the target and in the beam window, as well as heat load in the moderators.

Another parameter that can be optimised is the length of spallation material. The nuclear interaction length in tungsten is of about 10 cm. This means that in a few tens of cm most of the protons will have nuclear collisions, generating spallation reactions. Therefore, one does not need to have the full target wheel made of tungsten, but a lower amount. This is important since it can help in reducing the weight and the cost of the target.

Sensitivity to variations of engineering parameters. Already in the conceptual design phase the neutronic calculations contain engineering details; they are very helpful in determining the sensitivity of the results to the change in important parameters, such as the amount of structural material between target and moderator, or the distance between target and moderator. Concerning the latter, Figure 42 shows that the effect is not large, if the gap between target and moderator is kept within certain limits: increasing the gap by 1 cm decreases neutronic performance by about 2%. On the other hand, the reduction in heat load to the moderators is relatively large at 5-10% per cm, indicating that (if necessary) increasing the gap is a convenient way to control the heat deposition in the moderators.

Moderator. The dimensioning of the moderator was studied using MCNPX. Figure 43 indicates that the optimal diameter is around 18 cm for a conventional pure para-hydrogen moderator, although the loss in neutronic performance is not dramatic when a smaller moderator is considered. According to the size of the user demand for both thermal and cold spectra at the instruments, there is the option of a bi-spectral moderator, which allows the extraction of a wider neutron energy spectrum. Work is in progress to determine the optimal design of such a moderator for the ESS.

Another parameter related to the neutronic performance and the design of moderators is the dimension of the premoderators. In particular, the thickness of the water layer between the target and the moderator can help to reduce the heat deposition in the moderator, while at the same time improving its neutronic performance. Figure 44 reveals that thick ambient water premoderators placed between moderator and target can substantially decrease the heat load on moderators – by up to 25% – without compromising their neutronic performance.

3.3.2 Engineering design support

Neutronic calculations are important in support of engineering design for several aspects: heat deposition, gas production (H and He) and radiation damage to the TMR and monolith. Figure 45 shows the calculated energy deposition along three axes in the target geometry. Such calculations are used as input for the determination of the cooling requirements of the target. The quality of neutronic design clearly depends on the nuclear interaction models and nuclear data libraries employed. Comparison of different intra-nuclear cascade and evaporation models, evaluated data libraries and scattering kernels is under way. One example is shown in Figure 46. These results are of help to compile a set of rules and guidelines with regard to the use of various models and data libraries in TMR design activities.



Figure 43: Neutronic performance and moderator heat load as a function of the moderator diameter.



Figure 44: Neutronic performance in terms of cold neutron brightness and heat load on moderator versus bottom premoderator thickness.



Figure 45: Heat density along proton beam direction (Z axis), moderator axis (Y axis) and in perpendicular direction (X axis) normalised to 5 MW proton beam power.



Figure 46: Moderator heat load and cold neutron brightness in relative units obtained with different nuclear interaction models.

3.4 Beam extraction

3.4.1 Moderators

The ESS target station will have two wing geometry coupled liquid hydrogen cryogenic moderators with water pre-moderators, one above the target and the other below the target. Beamlines facing each moderator occupy two approximately opposite sectors of 60° . The two sectors on each sides of the target station will be positioned within 125° total range. Within each sector both the hydrogen moderator surface and the water premoderator surface can be viewed by each beamline for the extraction of cold and thermal neutrons, respectively, as illustrated in Figure 47. The viewed surfaces are 24 cm wide and 12 cm high.



Figure 47: Plan view sketch of bi-spectral beam extraction. The two outer guides are bi-spectral, while the central one is purely cold. Not to scale.

Optional enhancement of moderator emission. For enhanced cold neutron emission the liquid hydrogen moderator surfaces may be covered by a cooled beryllium filter-reflector, which substantially enhances neutron emission above a wavelength of 4 Å, at the expense of emission intensity below 4 Å. This enhancement method has been experimentally tested with success at the Lujan Center. Another method is to groove the viewed surfaces of the water pre-moderators, as tested with success at the pulsed neutron reactor at Dubna. Decisions on the optional use of these techniques will be made after in-depth neutronic studies, and after a complete analysis of instrumental needs.

Future moderator enhancements. The expected lifetime of moderators in the radiation environment of the target is estimated to be one to two years. Regular moderator changes permit the moderators to be continually re-designed for enhanced performance, as new developments become available and experimentally proven. It is assumed that such new developments will not be ready for implementation as part of the initial layout of the target; the development of the enhancement techniques at the Lujan Center and at Dubna have taken a decade. Nonetheless there is significant flexibility for improvements during the lifetime of the facility, following the current practice of some spallation sources.

3.4.2 Beamlines

The beamline directions are separated by $5.0 - 5.2^{\circ}$, making at least 50 ports potentially available at the target station. A 5° sector of the target monolith is exclusively reserved for each beamline, starting at 2 m from the monolith center. Parts of the beam extraction guides can reach closer to the moderator surface under the condition that they do not shadow the moderator and pre-moderator ensemble for the neighbouring beamlines, unless there is an approved agreement between the neighbouring beamline teams. The space reserved for each beamline houses the beam shutter and structural support elements of the monolith. It is 174 mm wide at 2 m from the center, and 523 mm wide at the outer edge of the monolith, 6 m from the center. The vertical dimension reserved for each beamline is 400 mm, eventually asymmetrically arranged, with at least 100 mm available both above and below the beam center. It is expected that about 4 instruments with short moderator-to-sample distances and substantial lateral dimensions will need to occupy 2 beamline slots at the edges of the 125° sectors. Neutron guides will be possible within the target monolith for all beamlines.

Bi-spectral beam extraction is optionally available in some or all of the four 60° sectors, providing the opportunity to offer both full thermal and cold neutron spectra in the same beamline and enhancing the

dynamic range of the instruments. The front end of such a neutron guide is broadened to about 160 mm at 2 m from the target station center. The number of bi-spectral beamlines actually needed will be determined as the instrumentation plans develop and the design features are refined.

3.4.3 Shutters, choppers, and neutron guides

Each beamline will have a beam shutter, sufficiently thick to allow unlimited hands-on access to the beamline when the source is not operating and the shutter is closed. Neighbouring beamline shutters must also be closed. The shutters could also be made sufficiently thick to allow work access when the source is in operation. This possibility will be studied later, together with the possibility of installing beamlines without shutters inside the monolith.

No choppers are envisaged inside the 6 m monolith radius. This assumption will be re-evaluated as the technology of radiation resistant choppers advances. The advantages of placing choppers closer than 6.1-6.5 m to the center have not yet been demonstrated, relative to the baseline multiplexing chopper systems that are consistent with established and experimentally tested chopper technology, and which are readily accessible outside the monolith.

Background reduction principles. The minimisation of the global neutron background is a common priority, facility-wide. The layout design of each beamline will be reviewed from this point of view by an appropriate panel. Advanced, supermirror-based neutron guides transport phase space distributions of cold and thermal neutrons with low losses over large distances to the sample. The following general principles are followed for each beamline, in order to avoid creating superfluous background:

- 1. The phase space volume extracted from the monolith shall not unnecessarily exceed the phase space volume that can be usefully accepted by the instrument(s) envisaged on that beamline.
- 2. The phase space volume permitting fast neutrons to escape from the target monolith shall be minimised.

Virtual source based beam extraction. The virtual source beam extraction technique is recommended in the design and evaluation of each beamline. It consists of concentrating the beam phase space volume to be extracted from the monolith into a well-shielded fast neutron diaphragm of minimal cross section, at a maximum distance from the moderators. This technique has been successfully implemented at several neutron sources, thereby reducing the fast neutron background.

3.5 Monolith and accelerator beam window

The monolith shown in Figure 48 is a vertical cylinder with the dimensions listed in Table 13. The monolith is located in the centre of the Target Station building, and is anchored into the basement slab (reinforced concrete above additional non-structural steel shielding), which assures a complementary shielding, in order to minimise as far as is reasonably achievable the soil activation under ESS facility. It contains:



Figure 48: Target Station monolith general view.

Irradiated and "short lived" parts. These components are designed to be replaced periodically in a normal maintenance period of the facility:

• Target wheel, the Premoderator, Moderator and Reflector plug (PMR plug), the Proton Beam Window plug (PBW plug).

Irradiated and/or contaminated "long lived" parts. These are the components that are designed for the 45 year duration of the ESS lifetime, but which could be replaced in a dedicated maintenance period if proven necessary:

• The 12 m diameter steel shielding inside the monolith liner (that is, its external envelop).

Parameter	\mathbf{Unit}	Value
Monolith external diameter	m	12
Monolith total height	m	12
Minimum thickness of the upper airplane crash absorber	m	1

Table 13: Monolith dimensions.

- The internal neutron guides facing the moderator surfaces.
- The shutters.

Upper Cells. These host the different circuits associated to the target, the PMR, PBW and shielding. These cells contain the interfaces with target station ancillaries (secondary cooling water circuits, HVAC et cetera).

3.5.1 Functions

The monolith is the shielding and the support of the activated materials during operation and maintenance, which are:

- tungsten,
- moderator $(H_2, D_2 \text{ or other moderator material for any kind of advanced moderator concepts})$, premoderator (water ...), reflector (beryllium, lead...),
- the internal neutron guides,
- steel and metallic alloys constitutive of the systems mentioned above participating to neutron production.

Parts of the monolith structures are classified according the zoning concept to address specific risks, such as:

- tritium zones,
- hydrogen zones,
- contamination and/or radiation zones (non classified, monitored, green, yellow, amber and red),
- any other specific risk, if relevant.

Among these zones, the main ones regarding nuclear safety are the contamination zones against target radioactive inventory, so called "safety barriers".

The monolith contains the first safety barrier against the target radioactive inventory. The monolith is also:

- the second safety barrier against the target radioactive inventory,
- the protective structure of the target radioactive inventory against external accidental situations such: airplane crash, earthquake, internal Target Station fire.

The second safety barrier is the external envelope of the monolith, including the following specific parts (from bottom to top):

- The barrier extensions to allow monolith draining (in the basement),
- The "neutron beam windows", which are replaceable parts, with low thermal and cold neutron absorption properties (such as zircaloy and aluminium alloys); they separate internal neutron guides and shutters from external neutron guides and choppers,
- The proton beam window and its extension to the connecting flange with the accelerator vacuum beam pipe,
- The external walls and ceiling of the different upper cells (doors, airlocks, circuit penetrations, openings)

Airplane crash protection is assured by:

- 1. An upper resisting structure absorbing energy and shock from the crash; typically, this is assured by a reinforced concrete structure of a minimum thickness of 1 m (see Table 13),
- 2. A lower layer (metallic protective drain) to collect and drain efficiently kerosene in order to evacuate fuel and limit fire effects on the first safety barrier.

3.5.2 Radioactive zoning and pressure cascade

The Target Station monolith participates in the radioactive confinement function. Its different volumes have a pressure cascade in a normal situation (power operation and maintenance) that is listed in Table 14. Figure 49 indicates the locations of the two safety barriers. The previous values are associated to the proposed values in Table 15, in order to keep a minimum pressure cascade between monolith zones and other volumes in the Target Station.

Parameter	Unit	Value
Internal monolith gas		Helium
Internal monolith pressure	hPa abs	991
Internal monolith free volume (incl. He circuit)	m^3	15 - 30
Upper cells atmosphere		Air
Upper cells pressure	$hPa \ abs$	$P_{atm} - 1.5$

Table 14: Monolith pressure cascade values – normal power operation.



Figure 49: Schematic view of the first and second safety barrier locations during normal power operation. The blue line indicates partially the first safety barrier (the fixed helium circuit connected to the target wheel is not drawn for clarity). The green line indicates the second safety barrier.

3.5.3 Loads and cooling

The following loads are to be considered for the monolith design. The final list will cover all situations listed in the Preliminary Initiating Events (PIE) list.

Pressure loads - normal situation

• Nominal cascade pressure plus margins² for continuous regime and internal vacuum loads for 45 years.

 $^{^{2}}$ Usually, margins integrate maximum pressure allowed by passive protection systems (if any) and first alarm defined in the control system

Parameter	Unit	Value
Instrument hall pressure	hPa abs	P_{atm} -0.3
Air pressure in Hot cells	hPa abs	P_{atm} -2.0
Target Station Basement pressure	hPa abs	P_{atm} -0.6
Target Station high bay area pressure	hPa abs	P_{atm} -0.6
A2T area pressure	hPa abs	P_{atm} -0.6

Table 15: Target Station building pressure cascade values – normal operation.

- Pressure resulting from accidental ruptures of the first safety barrier, of any of the PMR, shielding coolant and PBW circuits. All cases of vaporisation from leakages (hydrogen, premoderator water, shielding coolant, et cetera) are also considered. This design choice is made in order to keep the confinement function from the second barrier (the monolith envelope) even in case of severe scenarios. The replaceable PBW does not have to be designed for these overpressure scenarios, due to the fact that the expansion volume after rupture is confined in the accelerator vacuum vessel.
- Pressure resulting from accidental scenario on hot cell.

Pressure loads – accidental situations.

- Internal explosion from PMR plug.
- Partial tungsten melting proton beam continues at full power for a few seconds after coolant system failure. See parameters in Table 16.

Parameter	Unit	Value
Delay from request to proton beam shutdown – normal situation	ms	1
Delay from request to proton beam shutdown – accident	\mathbf{S}	2

Table 16: Parameter list for loading scenarios.

Thermal loads – normal situation.

- Full power mode, with normal proton beam shutdown time (see Table 16).
- Transient with total loss of power (several days).

Thermal loads – accidental situations.

- Temperature resulting from accidental delay of requested proton beam shutdown:
 - Internal explosion of moderators.
 - Reflector burning process (if any).
 - Internal TS fire (both from high bay area and from basement).

Mechanical loads (other than pressure) – normal situation.

- Handling accident with shielded cask (high bay area).
- Handling accident with shielding around extracted neutron beam (experimental level).
- Transient with total loss of power (several days).
- Foreseen earthquake

Mechanical loads – accidental situations.

- Airplane crash.
- Earthquake.

Cooling. Monolith coolant is assured partially by helium flow in free spaces between structures, and by active fluid loops (water or helium) in shielding.

3.5.4 Handling and interfaces

The following internal components are periodically extracted from, and/or inserted into, the monolith.

Short lived components

- PBW plug: vertically in cask, without helium replacement in the monolith. The monolith atmosphere and accelerator vacuum are maintained during PBW plug replacement in the following manner: Two valves are closed in the proton beamline, one upstream of the PBW and one downstream. Thereafter inflatable bellows are used to remotely disconnect two vacuum seals, one upstream and one downstream of the plug. Then the PBW plug can extracted vertically. The connection of the replacement is done similarly. The PBW plug also contains beam monitoring equipment.
- PMR plug (top and bottom PMR in a unique plug): vertically in cask, without helium replacement in the monolith.
- Target wheel and shaft (as a single block): vertically in cask, after PMR plug and shielding blocks have been removed. This operation requires helium to be drained from the monolith.

This last maintenance requires helium to be removed from the monolith and to have a different pressure cascade for the air in the different connected volumes (see Table 17).

Parameter	Unit	Value
Internal monolith gas		Air
Internal monolith pressure	$hPa \ abs$	P_{atm} -2.0
Upper cells atmosphere		Air
Upper cells pressure	$hPa \ abs$	P_{atm} -1.5

Table 17: Monolith pressure cascade values – normal maintenance operation.

Long lived components

- Any shielding block can be vertically extracted in a cask through an appropriate opening (for example, the PMR),
- Shutters are extracted vertically (see "Beam extraction" discussion),
- Neutron beam windows are disconnected and reconnected from monolith, from experimental hall.

All casks are transferred from the high bay floor to the hot cell ceiling.

Interfaces. As a consequence of the previous paragraphs, the monolith interfaces are described below. The monolith assures also confinement and shielding³ continuity with:

- The final part of the accelerator and associated components (neutron beam catcher, proton beam dump, proton beam-on-target diagnostics)
- The hot cells,
- The permanent circuit of internal monolith components (target wheel cooling circuit, PMR circuits, PBW circuit, shielding cooling circuit).
- The reinforced structural concrete supporting the monolith systems.

The monolith assures the confinement and shielding and neutronic continuity with the external neutron guides, the choppers and additional external shielding, all serving the different experimental areas.

Note for hot cell interface. As all internal monolith components are exchanged from it by vertical extraction from the high bay area and the upper cells, the hot cells are not necessarily connected to the monolith. The hot cell is indirectly interfaced to the monolith via the transfer casks.

³This function is also performed by "additional shielding" – see "monolith and shielding" discussion.

3.6 Remote handling and hot cells

The system of hot cells is designed to maintain, process, package and store used components and other waste items of the target station. The hot cells are built to prevent unintentional escape of radioactivity through the barriers provided by its design configuration and its contaminated waste/components management. Handling operations are performed remotely.

Dimensions and zones. The hot cell area is in close vicinity of (but is decoupled from) the monolith, in order to minimise handling. The three cells have different purposes, with full access in between them. During normal operation it will be possible to operate the different parts of the hot cells independently. The internal dimensions of the hot cells are described in Table 18.

Dimension	Unit	Value
Width	m	4
Height	m	5
Combined length	m	20

Table 18: Interna	d dimensions	of the	hot cells.	
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The hot cells and zones are:

- 1. **Maintenance cell.** This cell handles the primary waste delivered from the target station, mainly the target wheel, the PMR and the PBW. It will also accept more frequent low-activation waste, such as shielding, shutters, internal neutron beam guides and beam dumps. There will be roof access from the monolith high bay, and possibly also from the instrument hall for neutron beam guides. This cell will enable processing and maintenance of components.
- 2. Storage cell. This cell stores components that need to cool for some time before they can be handled further. It also stores components that are waiting for shipment to another facility. Components in storage flow both to and from the maintenance cell, and to and from the transfer zone and decontamination cell. This cell has the capability to store all types of solid waste. Depending on the size and need, this cell could be extended into the basement.
- 3. Transfer zone and decontamination cell. The decontamination cell is primarily used as a transfer zone through which new components such as target wheels and PMR parts are inserted into the other hot cells, and from which waste is shipped to outside facilities. More frequent human access to this cell enables maintenance on items and hot cell equipment such as the overhead crane. Component decontamination occurs in this cell.

Hot cell equipment. The primary equipment that allows used components to access the hot cells includes doors, windows, tele-manipulators (heavy and light), crane, controls, ventilation, and tools for maintenance, decontamination, and dismantling.

Test zone. A test and ancillary equipment zone is foreseen. This zone will be used to test handling equipment, physical interfaces, perform tests on spare new components, et cetera.

3.6.1 Functions

Hot cell functions are:

- 1. Used component maintenance and exchange (target, the Proton Beam Window, moderator plugs, et cetera).
- 2. Waste management (collection, storage, evacuation, et cetera).
- 3. Associated control system.
- 4. Power supply (electricity, water, compressed air).
- 5. Radiological safety (protection against irradiation, confinement, et cetera).
- 6. Contamination risk safety (protection against external or internal incidents, or accident events).

3.6.2 Loads.

The following loads are considered for the hot cell design. The final list will cover all situations listed in the PIE (Preliminary Initiating Events).

Normal conditions.

- 1. Hot cell internal pressures, relative to surroundings.
- 2. Pressure cascades and dynamic confinement during airlock operation.
- 3. Total thermal heat load (air cooling).
- 4. Protection against radioactive release.

Incident and accident conditions. Normal situation Thermal load coming from:

- 1. Overpressure protection.
- 2. Overheat protection.
- 3. Amount of combustibles and the expected heat load during fire.
- 4. Protection against radioactive release.
- 5. Maximum surface area accidentally exposed, through loss of shutters, window failure, et cetera.

3.6.3 Handling and interfaces.

Hot cell design is strongly influenced by the requirements of handling interactions with used target station components, waste, trash and containers.

Target wheel. Transported from monolith to hot cell via a cask. The wheel is first separated from the shaft. Shaft and wheel are transported separately, allowing for significant flexibility. For example, the wheel can be transported vertically in the hot cells.

Pre-moderators, moderators, and reflectors. The PMR plug includes a support structure or skeleton that is used both for handling and also to ensure calibrated positioning of the PMR in the monolith. PMR maintenance is performed in the maintenance cell, where it is introduced via the high bay.

Proton beam window. The size and weight of the PBW are not challenging for the hot cells. There is some need for maintenance and tooling to be able to reuse some structural parts of the PBW plug. Storage space will be allocated.

Neutron beam guides. Moved with a cask from the instrument hall, the neutron beam guides may be introduced either from the side or from the roof of the hot cell. Handling within the hot cell is being studied, for these delicate glass or aluminium alloy structures.

Miscellaneous. Handling requirements must also be established for the shutters, shielding, proton beam dump, neutron beam catcher and HEPA filters. It is also necessary to establish the irradiation plug function.

Interfaces. The hot cell interfaces assure confinement and shielding continuity with the monolith, the high bay casks, and the trucks and the handling system in the truck zone.

3.7 Ancillaries

Heat, Ventilation and Air Conditioning. Safety functions:

- Filtering of potentially radioactive exhaust gases
- Monitoring of activation of exhaust and ventilation
- Establishment of pressure cascading to support confinement of radioactive inventory

The Heat, Ventilation and Air Conditioning (HVAC) system(s) of the Target Station plays a vital role for minimising the radiological release to the environment and the public. They will be engineered for confinement and control of radioactive substances, both in full power operation and during maintenance situations. The HVAC systems will include so called HEPA (High Efficiency Particulate Air) filters that will efficiently capture particles, aerosols and condensable substances. HVAC will receive and treat off-gas from several fluid systems, like the pre-moderator circuits and shielding cooling circuits, as well as purged gases from for example the monolith, hot cells and utility rooms during handling and maintenance. All filtered off-gases and purged gases, as well as all other ventilation of the target station, will be discharged through a stack of appropriate height. The HVAC systems are also used to establish and maintain necessary negative pressure in for example the monolith and the hot cells during maintenance. Such negative pressure, or pressure cascading, is adopted for all operation modes and maintenance situations when needed to support and ensure confinement of the radioactive inventory. The HVAC systems are highly distributed systems that reach all areas and rooms of the target station.

Secondary cooling systems. Safety functions:

• Measurement of cooling temperature, flow rate and heat removal; as input to the control system of the facility

The secondary cooling systems will, by use of conventional water, serve the primary cooling circuits of all target components and transfer the heat to the ultimate heat sink, either to the district heating system in Lund or separate cooling tower. The secondary cooling systems shall be designed for a thermal load (heat removal) of 5MW during normal full proton beam power of 5MW.

Gas supply and storage. Safety functions:

- Treatment of hot off-gas, that is removal of tritium, noble gases and iodine where identified to be necessary
- Storage of gaseous waste during decay prior to controlled and monitored release to the discharge stack

The gas supply systems can be subdivided into supply systems for helium, nitrogen, hydrogen and compressed air. It is foreseen that all types of gases are provided to the target station either from centralised gas plants or tanks within the facility or by pressurised gas flasks. Utility rooms for gas supply systems shall be designed with sufficient pressure relief and ventilation equipment for conventional (personnel) safety. Treatment of gaseous waste is accomplished primarily by decay and filtering. Utility rooms for decay tanks, filters, adsorbers and re-combination tanks shall preferably be located as close as possible to the monolith and hot cells and in the upper levels of the facility.

Liquid supply and storage. Safety functions:

- Treatment of activated liquid drain, that is removal of tritiated water or other radioactive substances dissolved in the drainage.
- Storage of liquid waste during decay prior to disposal.
- Sampling of process drain prior to discharge to municipal sewage.

The liquid supply systems, primarily water systems, may be subdivided into systems for demineralised light water and conventional water for operational needs. For systems and components with heavy water requirements the supply of the liquid is preferably accomplished by mobile tanks. It is foreseen that all other types of liquids are provided to the target station from centralised tanks within the facility. Water processing and re-processing systems may be located either in the basement or in higher levels of the target station. Liquid drain from process systems; for example condensate from filters and HVAC, floor drains and drains from water cooling systems; will be collected in a sump and sampled for potential contamination before discharge to the municipal sewage. If any contamination is detected the collected drain liquid will be redirected to storage tanks for active liquid waste. Utility rooms for drain tanks, sump and storage tanks for active liquid waste may be located in the target station basement.

Fire protection system. Safety functions:

- Detection and extinction of fires in cells and rooms that contain the radioactive inventory, radioactive waste or contaminated substances
- Personnel protection

The fire protection system consists of one part for detection and one part for extinction of fires. The smoke detection systems together with air sample detectors are designed to detect early and warn in case of a fire. Either a water mist or a water sprinkler system may be envisaged for different areas of the target station, depending on the specific requirements. Special requirements apply for rooms and areas containing radioactive inventory, for example hot cells, radioactive waste, for example decay tanks, or contaminated substances, like HEPA filters. Dedicated fire protection systems shall also be considered to ensure the integrity of radio-protection barriers as well as to secure operability of systems for radio-protection also require dedicated fire suppression equipment, for which halogen extinguishers may be considered. Operability of the fire protection systems may be required for a specified time also in case of a loss of power supply globally to the facility or locally to the target station or its sub-systems. The fire protection systems are highly distributed systems that in principal shall reach all areas of the target station.

3.8 Materials and lifetimes

The ESS Target Station will contain a wide range of materials, serving various functions under very different environments. Materials considerations for components of the Target Station are driven by a need to support the mission and responsibilities of the ESS project:

- safety: ensuring the target station is engineered for safe operation and for predictable behaviour during operation, incidents and accidents.
- maintainability/availability: interventions on activated components inside (or outside) the target station are generally complex and must be minimised.
- cost: material costs associated with components of the target station including spares, maintenance and disposal costs.
- scientific performance: optimising materials especially in the target/moderator/reflector area will play a crucial role in increasing neutron yield.

On the basis of the above-mentioned factors, materials can be classified according to a number of categories:

- Permanent versus replaceable components
- Structural vs non-structural
- Safety function vs no safety function
- Highly activated vs lightly activated

Here, the focus is on critical components close to the proton beamline, exposed to the harsh radiation environment, high heat loads and operating under very specific conditions such as the spallation target and the cryogenic moderators. The properties of fluids are not discussed in this section.

3.8.1 Structural materials

Several structural materials, mostly steels, have been extensively studied for applications in reactor environments and to a more limited extent in spallation neutron sources. The cycle for full qualification of a material exposed to a radiation environment involving manufacturing/metallurgy, mechanical and chemical properties determination typically takes years (5-20 years). Whilst the development of an entirely new structural material for the ESS target can be foreseen, it is likely that it will not be ready before first beam on target scheduled for 2019. The structural material for the first target (target changes will occur with a low frequency) will be chosen from a list of totally or partially qualified materials for which extensive experience has been collected at the various spallation sources built and operated in the last decades, or for which confidence can be drawn from similarly proven structural materials applied under similar conditions. Standardised design codes will be used, wherever applicable, for quality assurance and safety.

Structural material candidates. The main candidate structural materials for critical ESS Target Station components are stainless steels such as SS316L(N), martensitic steels such as T91, aluminium alloys such as Al6061-T6, zirconium alloys such as Zircaloy 4 and Titanium alloys such as Ti6Al4V. In the short term, materials will be selected based on experience from previous spallation facilities: stainless steel for the target envelope and shielding vessels, aluminium alloys for the moderator and reflector vessels and the proton beam window. Eventually other materials could be considered such as Zircaloy for the moderator external envelope or Ti6Al4V for the target envelope or proton beam window.

Applicability of nuclear pressure vessel design codes to the spallation domain. We are reviewing the forthcoming RCC-MRx (planned for 2012) design code and assessing its applicability to the spallation domain. The motivation is two-fold:

- to use it to design safety-credited structures,
- to design other structures when required, using rules coherent with the code.

A full "radiation" mapping of the target station is planned which will indicate fluxes and energy spectra for each particle type. A careful analysis of this map will be required to determine which structures can be designed with the code. It must be noted that structures not directly exposed to incident proton primaries could be exposed to a radiation field not covered by the code such as high-energy neutrons or secondary protons. In order to gain an insight into the structure of the code, the origin of criteria for the selection of material data must be understood. Once the criteria have been explored, the damage modes in the spallation domain should be compared to the fission domain to identify any differences.

Although access to the original data used to set up the RCC-MRx code is mostly restricted, first indications are that they are from a variety of radiation tests with often very different radiation characteristics. However different these radiation environments are though, none approach the high levels of hydrogen/dpa or helium/dpa of the spallation domain which lead to faster embrittlement and loss of ductility in steels for example.

To enable a staged approach where components exposed to a radiation environment at ESS not currently covered by the RCC-MRx code, could nevertheless be designed with "best practice" rules coherent with the code, it is proposed to establish a "code case". This would be dedicated to the ESS spallation environment and its scope of application could be extended to more generic conditions, such as: proton irradiation, high energy neutron irradiation, damage by high production rate of transmuted gas (He, H). Its structure should be built with irradiation experts, to define for each material: the relevant parameters to describe irradiation effects, the borderlines, and the dedicated design rules for significant neutron-proton mixed spectra.

3.8.2 Non-structural materials

The most critical non-structural material is the spallation material itself: it is the largest source of the ESS radioactive inventory and must operate reliably and predictably for the planned lifetime of the target. Amongst the potential candidates for a helium-cooled rotating target, tungsten and its alloys are retained as primary candidates. Furthermore, it is foreseen to focus on pure tungsten during the TSDU project phase. This decision is based on extensive experience from the fusion community in attempting to identify or develop alloys with better properties than those of pure tungsten and reaching the conclusion that pure tungsten offers the best set of properties. Knowledge of the evolution of tungsten properties under irradiation is limited.

Thermo-mechanical properties of irradiated tungsten. Knowledge of how thermal properties (thermal conductivity, heat capacity, emissivity) and mechanical properties (thermal dilatation, Young modulus, Poisson ratio, tensile strength, fatigue, hardness) evolve with temperature and irradiation is important at an early stage, especially when thermo-mechanical studies are being carried out to dimension the target system.

Starting an irradiation program during the TSDU or P2B phases is unlikely to yield results in time for the design phase. By searching for tungsten that has already been irradiated in a spallation environment and with a level of activity, which has been allowed to decrease in time, it is possible to ship it and test it in time to obtain valuable data for the design phase. The following facilities are likely to have a significant inventory of irradiated tungsten:

- ISIS RAL UK
- ISOLDE CERN CH
- LANL US

Potential ESS partner institutes where these studies could be performed include Halden, Studsvik, and PSI. Dedicated future irradiation programs are required to establish in detail the behaviour of tungsten under representative operational conditions, for example with the correct volumetric energy density, temperatures and coolant pressure and flow rates. Planned future irradiation programmes at the PSI SINQ facility, the Spallation Target Irradiation Programme - STIP, offers the opportunity to control many of the irradiation parameters.

Release of isotopes from tungsten. The release properties of tungsten, characterised by diffusion through the bulk material and desorption from its surface, should be studied in detail over a wide range of temperatures:

- to estimate contamination and activation of the helium loop, as an input for loop components such as filters.
- to estimate consequences of various accident scenarios, required for mitigation strategies during design and for licensing.

The ISOLDE facility at CERN offers the possibility to quantify radioactive isotopes released from the target during operation. Thin 20 μ m tungsten foils are already used at ISOLDE to produce radioactive isotope beams. These targets could be adapted for the ESS study by varying for example the thickness of the foils. It should be noted that in the 1970's and 1980's comparative studies of hafnium, tantalum and tungsten showed diffusion coefficients for rare earths of 10^{-7} cm²s⁻¹, 10^{-9} cm²s⁻¹ and 5×10^{-12} cm²s⁻¹ respectively, at 2000°C. This
indicates that tungsten is not the best of materials for release properties especially at around 500°C operation temperature. Hence short-lived isotopes would most likely decay within the tungsten bulk.

Radiochemistry expertise exists within the ESS collaboration to quantify release from tungsten through tests post-irradiation for long-lived isotopes. The slip-clad tungsten rods irradiated at LANL offer the possibility of testing the composition of the gas filing the space between the tungsten and the steel cladding. The proton fluence on these LANL rods exceeds that of ESS, and therefore is representative of what can be expected for maintenance or decommissioning.

Helium-tungsten interaction – cladding. The cyclic thermal loading of tungsten in a rotating target configuration at ESS and the use of helium as a coolant at high flow rates and pressures call for a better understanding of "surface" effects in a spallation environment. Any surface imperfections can be the sites of crack initiation, leading eventually to fracture and loss of integrity of a tungsten component. Surface erosion can lead to activated tungsten dust being carried in the helium stream, eventually collecting in unwanted areas of the helium loop. ESS has had exchanges with experts in the fusion domain from FZJ, ITER, KIT, and following TAC recommendations has contacted the EFDA Plasma Wall Interaction Task Force. The fusion community has investigated several surface phenomena, establishing thresholds for the onset of blistering and sputtering as a function of incident particle type (hydrogen, deuterium, helium), energy and tungsten temperature. The penetration depth of these particles during tests is in the range of a few nm. When converting the high surface fluxes to volumetric particle densities and comparing to the spallation environment (densities of hydrogen and helium), there is a factor of 10^6 difference, that is spallation conditions are well below thresholds for the onset of blistering/spluttering. Nevertheless, a better understanding of the diffusion of radiogenic species from the bulk tungsten towards its surface and of their desorption from the surface is required. Techniques and tools developed by the fusion community could be adapted for that purpose. ESS can also benefit from the extensive experience developed by the fusion community in alloying and manufacturing tungsten.

One of the main advantages for helium-cooled targets is the possibility to eliminate the cladding. Investigations of helium-tungsten interactions under operational conditions will determine whether the data obtained give enough confidence to commit to a start-up or production ESS target. In parallel to these investigations, cladding techniques must be evaluated and will be considered the most conservative choice since there is a lot more experience of operating tungsten clad with typically tantalum, stainless steel or zircaloy under a spallation environment. The motivation for the cladding there is that previous/existing systems were/are water-cooled. The slip-cladding technique investigated at LANL offers a good starting point for investigations of cladding.

The use of cladding introduces additional issues such as:

- irradiation effects on mechanical properties/microstructure of cladding materials.
- irradiation effects on bonding between tungsten and cladding. This applies in the case where there is direct bonding, not necessarily for slip-cladding.
- Compatibility of cladding material with helium coolant.

3.8.3 Lifetimes

An estimation of the lifetime of components is required to establish maintenance scenarios, plan for spares, build in an upgrade strategy and estimate costs. The evolution of material properties with irradiation is to be combined with "best practice" rules described in design codes such as the RCC-MRx to determine allowable design margins and hence up to which radiation dose a particular component can be exposed. The failure of other components functionality within the rotating target, such as monitoring devices could lead to shorter lifetimes than the substantial increase predicted by irradiation damage alone. Final estimates for the lifetime of components will be one of the main subjects of the TSDU, and will require setting a certain number of variables such as proton beam profile, materials and geometry. Nevertheless, it is possible to extrapolate from previous studies such as those performed for JSNS, where the 3 GeV beam energy is the closest to the 2.5 GeV ESS proton beam. Taking an SS316L static target envelope, the estimated damage rate is 20 dpa/year for a 5 MW beam and 5000hr of operation corresponding to 0.5 dpa/year for a rotating target. Although it is far from being confirmed, especially if the target envelope is safety credited, we will assume here an acceptable maximum dpa level of 5 dpa leading to a 10-year lifetime for a 2.5 m diameter target wheel. A similar exercise would lead to a lifetime for the aluminium alloy moderator and reflector vessels of just over 1 year, if an acceptable maximum dpa level of 20 dpa is assumed. Here the unit used is already an indication that some work is required to bring lifetime estimations inline with pressure vessel codes where the lifetime for aluminium alloys is expressed in terms of percent silicon content produced by irradiation.

3.9 Shielding and activation

Shielding in ESS will be designed and engineered to ensure that radiation exposure is as Low As Reasonably Achievable (ALARA), but complying with the standard radiation levels.

Preliminary analysis of the photon energy spectra from the activated target components at shut-down after one year of operation was done for a mercury target, as shown on the left of Figure 50. One can see that if for the target the gamma rays have an average energy of about 0.2 MeV, for other components the photon spectra are harder. The wide line in the energy bin around 2 MeV in the moderator cladding is due to ²⁸Al while the strong photon peak between 6 and 7 MeV comes from ¹⁶N inside the premoderator. Therefore, the hard gamma ray coming from aluminium cladding and cooling water surrounding the moderator will be important issues for the optimisation of the shutter thickness. After a shut-down the total gamma strengths decay away, as shown on the right of Figure 50.



Figure 50: Photon emissions from various activated target assembly components. Left: Photon energy spectra at shut-down. Right: The total gamma source strengths versus decay time.

An optimum in terms of shielding performance as well as cost of merit will be determined. Investigations to find out the optimum position of the neutron beam shutter are needed.

3.9.1 Environmental compliance

Soil activation and potential groundwater contamination. For environmental safety the activity concentrations in soil and groundwater under the target station are very important. Concentration levels that would reach the public water supply are based on the source term derived from the soil activation calculations. Thanks to the heavy shielding to be applied (about 5 m of iron followed by heavy concrete) the soil activation levels are small compared to the estimates for the ESS accelerator [70].

Production of gaseous elements during operation. An estimation of the possible emissions from the ESS system requires knowledge of the amount of volatile nuclear reaction products that might be released from the target. The gaseous elements produced in tungsten targets were calculated at various operation times up to 5000 h, as shown in Figure 51. The linear increase of the gas concentration with the irradiation time is obvious from the figure. The total amount of non-reactive gases produced in the target within the timeframe of a campaign defines the capacity of the gas extraction system.

In order to judge the estimated production values in terms of the potential impact upon the environment and to establish a scenario of the ³H release into the atmosphere it is usually useful to compare directly the production obtained with the authorised release limit. In Swedish legislation there is no stipulated limit for ³H release. According to the Swedish law [71], for activities where the gaseous radionuclides are produced or generated from the system with known radioactive substances, their contribution to the dose for a representative person must be estimated. This estimation should be based on a documented methodology of the calculation of the correlation between released activity and effective dose. The operator has an obligation to report the amount of released activity per radionuclide each year. If emission to the air, estimated as described above, causes annual effective dose of 10 μ Sv or more per representative person, a realistic calculation should be performed and documented.



Figure 51: Gas production as a function of the irradiation time of the tungsten target.

The most conservative approach is the direct calculation of the effective dose from the ³H activity produced in the target multiplied by the committed dose coefficients. This rough approach leads to overestimated effective dose values for the committed dose from inhalation exposure. Therefore more realistic calculations are required, using site-specific data. Obviously not all amounts in the table will be released, especially from the solids. The emission of ³H should be considered regarding its release through the off-gas system. As a final concluding remark, ³H is almost irrelevant in assessments of the radiological impact of activated air due to its decay channel (weak beta).

3.9.2 Total activity in the target moderator and reflector assembly

Activation calculations for the tungsten target have been performed using the Monte Carlo code MCNPX to simulate spallation reactions induced by the proton beam on the target and to transport the generated particles. The output from MCNPX (isotope yields for energies > 20 MeV and neutron and photon flux for energies < 20 MeV) was used with the CINDER90 code to calculate the residual activity of the target. A calculation model of the ESS target moderator and reflector assembly (TMRA) was developed using geometry parameters taken mainly from McManamy [72], where a long-pulsed TMRA model was optimised. The geometry model used in calculations is given in Figure 52. Calculations were performed up to the life time of the target, considered to be 5 years for tungsten target material with the irradiation conditions simulating the overall irradiation history of the facility by 3 years of continuous operation with a duty cycle of 0.57 (5000 hours per year) and subsequent 2 years with partially full power, having a shut-down period in between.

The results of the calculations after 5 years of irradiation are presented on the left of Figure 53. The graph shows the total induced activity together with its main contributors as a function of the decay time. For decay times less than 1 year the total activity in the tungsten target is driven by the tungsten radionuclides 187, 183^{*}, 185, and 181, followed by ¹⁸⁶Re, ¹⁸⁸Re and ¹⁷⁸Ta, and ¹⁷⁹Ta. At shut-down ¹⁴⁸Gd represents less than 0.1% of the total activity. After 1 year decay time tritium gives an important contribution in the target material. Decay heat results obtained are given on the right of Figure 53.

The tungsten target integral decay heat at shut-down is higher than that reported for the SNS 3 MW rotating target [72]. Reasons for this difference are under investigation. Since maximum heat density is important for thermal hydraulic design, the detailed spatial distribution of the decay heat has to be estimated for the optimised neutronic model of the tungsten rotating target. The dominant contributors to the total decay heat at shut-down are: ¹⁸⁷W, ¹⁸³*W, and ¹⁸⁸Re. Decay heat generated in the structures of the TMRA was also calculated, giving the decay heat concentrations. The decay heat density was derived considering a tungsten wheel volume of 120.6 litres [73].

Similar calculations have also been performed for the comparative target material lead bismuth eutectic, with results showing similar levels of radioactivity after a comparable operational activation.

Waste characterisation. In the assumption that the entire energy generated by decay is transferred to the material, the decay heat gives the level of the thermal power in the target, an important parameter used for the classification of the radioactive waste. According to IAEA recommendations on the safety of radioactive waste management, 6 waste categories are defined and must be used as the basis for the waste classification [74, 75].



Figure 52: TMRA geometry model used in simulations. Left: View of the MCNPX model in the mid-plane (top), and in the opening plan (bottom). Right: Side-view of the MCNPX model in the OX=0 plane (top), and a detailed model of the moderator in the plan OZ=0 (bottom).



Figure 53: Target behaviour as a function of the decay time after final shut-down. Left: The total induced activity and the main contributors. Right: Total decay heat and dominant constituents.

In the frame of the IAEA rad-waste classification the high level waste (HLW) is defined as the waste containing a large concentration of both short and long lifetime isotopes such that it generates significant quantities of heat from radioactive decay for a long time period. An irradiated target is in the HLW category after its operational lifetime is over.

Waste management. Transportation of the HLW has to meet the IAEA requirements for the safe transport of radioactive material [76]. The high level of activity in both types of target suggests that shortly after the shutdown the target might be transported as a type C package as defined by the IAEA regulations. Both terrestrial transportation and dismantling of radioactive wastes at high levels of activity and thermal heat require special attention and additionally incur supplementary costs. So far there is no Swedish experience in this respect [77]. Usually the spent fuel from nuclear reactors that might be HLW is stored in pools until the activity reaches levels allowing transportation and disposal. Due to these restrictions related to the transport/disposal of the HLW the storage of the spent target on the ESS site prior to disposal might be the preferred solution. On-site storage is recommendable especially in case the solid target, at the end of irradiation, has to be treated as operational waste.

In agreement with the results obtained it is recommended to store the spent tungsten target on the site for about 5 years until the activity and consequently the after-heat have decreased to permissible levels. Therefore an adequate storage room having capacity for at least two tungsten targets is required. At least four spent tungsten target may be produced during the 45-year lifetime of the facility. Similar analyses as above may be done for the TMRA structures. The results of the thermal heat concentrations in stainless steel shrouds and aluminium cladding of the moderator show that for the stainless steel shrouds more than 1 year decay time is needed until the concentration of the thermal heat drops below the threshold set for the HLW classification. Nevertheless the lifetime of the stainless steel material used for shrouds under the operational conditions of both target concepts has to be defined in order to decide the irradiation history upon which these shrouds are defined as radioactive waste and further classified.

Similarly for the aluminium cladding of the moderator where the calculations performed for an operation time given by the target lifetime lead to the conclusion that in the case of tungsten concept a waiting time of about 1 week is required before transportation As above the lifetime of the aluminium cladding has to be defined and consequently a real analysis of the waste arising from this item needs to be performed.

Storage and disposal. Considering the constraints related to planning for ESS decommissioning of the ESS installation as shown in Figure 1, and the fact that ESS has rented the land until the year 2108, a better choice might be a temporary storage in the in-building hot-cell allowing the decay of the activity and heat and subsequent transportation as HLW to the Studswick site for further storage until the thermal heat decreases below the limit of 2 kW/m³. Obviously this solution increases the decommissioning cost and requires early preparation of the target storage/transportation strategy (design and licensing of the transportation container).

Preliminary decommissioning plan. The straightforward option for decommissioning the ESS facility is immediate dismantling. However it is a general requirement that an initial decommissioning plan should consider other options as well, such as various models of deferred dismantling. In general, the main differences between these main options are given by the following parameters: time requirements, end-points, dose exposure to radiation workers, dismantling technology, waste management costs, decay storage, expertise. These aspects will be elaborated and analysed in detail by the team responsible for submitting the licensing documentation.

3.10 Tune-up dump and irradiation ports

3.10.1 Tune-up beam dump

The tune-up beam dump for the proton beam is located in the direction of the beam but not necessarily on the same level. It is used for day-to-day tuning of the beam before the beam is sent to the target. The tune-up beam dump is situated in the target building and the engineering of the tune-up dump is therefore a scope of the target design. Figure 54 shows a schematic picture of the beam dump setup. This solution is considered to be the one with least risk since the accelerator is pointing in the direction of the dump.



Figure 54: Schematic drawing of the tune-up beam dump.



Figure 55: Schematic drawing neutron beam catcher.

Parameters. The dump includes a simple quadrupolar expansion system to enlarge the proton beam cross section in order to reduce the cooling issues of the dump. The tune-up dump is relatively small, and under normal operation it will only see a reduced beam power. This is obtained by a combination of a lower repetition frequency and a shorter pulse length. Under an abnormal event the beam dump should be able to handle two pulses of full length with full beam power. Parameters of the tune-up dump are listed in Table 19. The proton beam dump will last the lifetime of the facility, although it will be possible to perform maintenance during this time. A shutter system is therefore included between the tune-up dump and the accelerator.

Parameter	Unit	Value
Minimum beam cross sectional diameter at dump	$\mathbf{m}\mathbf{m}$	50
Normal operation power	kW	50
Repetition frequency	Hz	1
Pulse length	\mathbf{ms}	0.4

Table 19: Proton beam tune-up dump parameters.

Materials. The tune-up dump core is either graphite or copper, followed by an outer heavy material region to absorb the power and secondary particles. A thin window is placed at the entrance of the dump, separating the "clean" vacuum of the accelerator from the "poor" vacuum of the tune-up beam dump environment. This thin window is made of steel, aluminium, or Zircalloy.

Design. The tune-up dump is cooled by helium. The system is accessible for maintenance, either in place or via a plug construction to the high-bay area. The shielding nearby the dump assembly is thick enough to reduce radiation to fulfil the requirements of the GSO. A thorough calculation of the tune-up beam dump design has yet to be performed, including cooling capability, transient thermal loading and structural design.

3.10.2 Neutron beam catcher

The purpose of the neutron beam catcher is to absorb back-scattered fast neutrons from the target, as sketched in Figure 55. The design includes a passive system and a metal plate to absorb the neutrons. The plate thickness and design depend on the distance to the target and the results of neutronic calculations. The shielding around the neutron catcher system is thick enough to reduce radiation levels to fulfil the requirements of the GSO.

Parameters. The neutron catcher will last the lifetime of the facility, although it will be possible to perform maintenance during this time. A shutter system is therefore included between the catcher and the accelerator.

Materials. Studies performed at other facilities show that a combination of layers of concrete and steel efficiently capture backscattered neutrons. These materials are used as a baseline.

Design. A passive system using helium cooling is the baseline choice. Water-cooling is an alternative option, since the deposition power is much less than in the tune-up dump. A tunnel may be included in the layout, to decrease the backscattering from the neutron catcher.

3.10.3 Irradiation facilities

The thermal and cold neutron spectra generated by the target, pre-moderators, moderators and reflectors are the main goal of the ESS. In addition, fast neutron spectra (possibly mixed with proton spectra) will be extracted from the monolith, in order to irradiate samples and components. The first and main goal of these irradiation facilities is to test material and systems for ESS operation under ESS-specific conditions, both for safety and reliability. The list of materials and systems potentially concerned includes:

- 1. Structural or non-structural materials for the monolith systems, irradiated with 2.5 GeV protons and neutrons:
 - (a) Target material.
 - (b) Target container and structures.
 - (c) Moderator material.
 - (d) Reflector materials.
 - (e) Sensors, including electronics located in the target neutron flux.
- 2. Electronic, optoelectronic and microelectronic equipment subjected to the radiation field, ionising doses or displacement per atom (by fast neutrons and/or by protons). Tests would investigate the behaviour of equipment such as Single Event Upset, background noise generation and other failure modes.

Various representative operating conditions (such as temperature or pressure) will be adjustable, in order to qualify materials and components.

The target station conceptual design includes two types of irradiation facility:

- 1. The proton beam dump shown in Figure 56, located at the end of the linac, receiving proton fluxes during accelerator tune-up, typically receiving a 50 kW proton beam for a few weeks per year.
- 2. Fast neutron ports located in the monolith, with two potential locations shown in Figure 57. The first location is in the High Energy Beam Transport (HEBT) zone, accessible in the transition between the accelerator and the monolith, where backscattered fast neutrons from the proton beam strike a hot spot on the rotating target wheel target in a direct view. The second potential location is in the forward direction behind the target wheel, benefitting from the highest energetic shower of particles generated.

Beam dump location. The beam dump will integrate removable sample supports, taking into account cooling ability, manufacturing, handling, and shielding.



Figure 56: Proton beam dump and neutron beam catcher in the target station building.



Figure 57: Two potential locations for fast neutron ports. Left: In the High Energy Beam Transport zone. Right: In the forward direction.

HEBT zone. The fast neutron port shown in on the left of Figure 57 is located in the proton beam horizontal plane, in a backward direction at an angle of about 163 degrees with respect to the proton beam axis, in order to disturb neither the neutron guides nor the target handling. It has a direct view of the proton beam footprint on target. This port goes through an opening in the moderator plug, inside the beryllium reflector, down through the permanent shielding blocks, and through an opening in the monolith shielding, down to the monolith envelope. The opening in the monolith shielding and in the reflector allows samples to be placed at various distances from the target wheel. Handling is done from the HEBT zone during beam shutdown periods, in the vicinity of the neutron beam catcher shown at the right of Figure 56. Adjustable shielding downstream of the samples on the irradiation port line protects the monolith envelope window. This irradiation port window potentially contains penetrations for on-line monitoring of irradiation conditions (gamma and neutron doses, temperature, et cetera), and of fluid circuit penetrations, permitting the sample temperature to be adjusted during irradiation.

Forward direction zone. The fast neutron port shown on the right of Figure 57 is located close to the forward direction with of the proton beam axis, going through an opening in the monolith shielding, down to the monolith envelope. It does not disturb the neutron guides or target handling.

Investigations on irradiated target structures. The design of removable irradiated components (such as a target, PMR plugs, PBW plug, and shielding) will include the ability to retrieve samples after their dismantling or during their maintenance phase in the hot cells, in order to monitor irradiation damage. This will provide important information for improving the design and lifetime of regularly replaced target sub-systems, over the 45 year lifetime of the facility.

3.11 Upgradeability

The performance of ESS for neutron scattering experiments is primarily determined by the peak brightness of the neutron moderators during the long pulses and the total number of neutrons per pulse. The relative weight of these two key parameters varies between different types of experiments. The peak brightness is proportional to the proton beam current during the pulses, which is the most challenging feature of the accelerator. The other key parameters of ESS, such as the proton energy, the pulse frequency, and the pulse length have been optimised with the purpose of providing optimal performance and cost benefit ratio for a fixed peak proton beam current (actually 50 mA). It is expected that by accumulating operational experience with the ESS accelerator it could become possible in the future to enhance this peak proton current (and eventually also the final proton energy) while keeping all other pulse parameters fixed. This preferred upgrade path will maintain the ESS operational parameters as optimal for a fixed proton beam current. It implies for the target, enhanced activation, enhanced heat deposition, enhanced cooling needs and reduced life-time of some components due to enhanced radiation damage.

Enhanced activation of the target increases the decay heat developed after shutting down the accelerator. This after-heat represents the most challenging safety issue for ESS in case of an electric power cut which implies loss of cooling for the target without the implementation of expensive (and never 100% failsafe) emergency backup power systems. The ESS target is designed to require no backup power, or emergency cooling in case of loss of cooling at full facility shutdown after 5 MW proton beam power operation for any length of time. The maximum temperature inside the tungsten target will reach less than 500 C under the effect of the after-heat, which initially decays in time with a time constant of approximately 3 days. The structural stainless steel parts of the target wheel will reach about 400 C. With the low chemical activity of the He gas coolant, in this kind of temperature range no chemical reaction takes place between target, stainless steel and coolant, and the structural solidity of the target system also is not compromised before reaching much higher temperatures. This leaves sufficient margin for a substantial increase (at least doubling) of the ESS proton beam power both for the stability of the target material in the stagnant He atmosphere, and for avoiding rapid structural damage to the supporting structure.

Cooling of the target under higher heat deposition by the proton beam seems to be the most challenging target upgrade issue. We are expecting about 500 C maximal temperature during operation inside the most exposed tungsten blocks. Therefore there is room for increasing the operational temperature. Further power potential is offered by enhancing the coolant flow rate for more cooling power. The lifetime of the rotating tungsten target is expected to exceed 5 years without loss of integrity. More frequent exchanges (such as 2.5 years) could be envisaged, if necessary, in order to take account of the eventual reduction in structural material lifetimes under higher radiation damage and increased fatigue. Stress and fatigue is being kept under control by the wheel-type target design, in particular by reducing the thermal cycling rate to 1/3 Hz. The granular character of the target material is aimed at low stresses, and the low inertia and rapid response capability of the He cooling system allows for reducing the main common source of fatigue, the rapid cooling after frequent trips of the accelerator power. These potential modifications of the operational conditions will be primarily based on accumulated experience during the first couple of years of full power ESS target operation. Together with appropriate investments in higher power cooling equipment (pumps, heat exchangers, cryoplants for the moderators), they can be expected to allow for at least doubling the beam power on target and the peak neutron brightness of the neutron beams without modifying the target station and its lay-out, with the exception of the components that need regular replacement (target, moderator-reflector plug, proton beam window).

Another path of upgrading the neutronic performance of ESS is to improve and optimise the efficiency of the moderators in order to convert a higher fraction of the originally produced fast neutrons into slow neutrons emitted to the beamlines. The regular (about yearly) replacement of the moderators due to radiation damage will offer opportunities to keep improving the moderator-reflector system over the full lifetime of the facility. There are a number of new target materials and new target geometrical lay-outs proposed worldwide more or less recently, which might lead to substantial improvements on the time horizon beyond 2025. Recent successful examples (for example cold moderators with Be filter-reflector) have shown that such new developments require about a decade from conception to actual installation for regular use at a productive neutron source facility.

In sum, by the combination of operational experience, development of the regularly replaced neutronic components and installation of enhanced cooling capabilities in the target utility area the upgrade potential of the target performance in terms of neutron intensity on the samples is expected to exceed a factor of two without modification or exchange of the permanent structures in the target station, that are not regularly replaced anyway in normal operation.

4 Accelerator

4.1 Overview

Generally it is agreed that a proton kinetic energy of 1–3 GeV is optimal for practical target and moderator designs, and to keep the shielding requirements reasonable. The ESS energy of 2.5 GeV requires an average macro-pulse current of 50 mA to reach a beam power of 5 MW. This current is consistent with the need for high reliability, but leaves some leeway for a potential energy (and thus power) upgrade. The current limit is mainly set by space charge effects at low energy, by the power that can be delivered to the beam in each cavity at medium and high energies, and by beam losses. The ESS has the ambitious goal of being a sustainable research facility with net zero release of carbon dioxide. This will be achieved through a combination of actions, primarily focused around the most energy-hungry component, the linac. Care is being taken to optimise the overall energy efficiency, and to re-use the hot water coming out of the facility.



Figure 58: Block diagram of the HS_2011_11_23 layout of the ESS accelerator. The orange items (such as the Radio Frequency Quadrupole and the Drift Tube Linac) are normal conducting, while blue items (the spoke resonators and the medium and high beta elliptical cavities) are superconducting.

The general lay-out of the ESS linac in the HS_2011_11_23 configuration is shown in Figure 58. The proton ion source is a compact Electron Cyclotron Resonance source (ECR) similar to the VIS source [78] in Catania, and to the SILHI source [79] at CEA Saclay. The beam from the ion source is transported through a Low Energy Beam Transport (LEBT) section to the Radio-Frequency Quadrupole (RFQ) for bunching and acceleration up to 3 MeV. The RFQ is of the four vane type [80]. A similar RFQ, IPHI, which is presently under commissioning at CEA-Saclay, will be tested with realistic ESS performance parameters. The beam is transported from the RFQ and matched to the normal conducting Drift-Tube Linac (DTL) through a Medium Energy Beam Transport (MEBT) section. It is not yet decided if the MEBT contains a fast chopper.

The first superconducting section contains double spoke resonator cavities that take the 50 MeV beam to 191 MeV. Spoke resonators have a large transverse and longitudinal acceptance over this energy range. They are mechanically much stiffer than elliptical resonators, reducing their sensitivity to microphonics and to Lorentz force detuning. The spoke resonator section is followed by two families of elliptical cavities. The first takes the beam to 653 MeV, and the second to the full energy of 2.5 GeV.

Accelerator parameters. The HS_2011_11_23 layout sketched in Figure 58 is described in somewhat more detail by the lattice parameters listed in Table 20. High level parameters such as the 5 MW beam power already listed in Table 2 are rigidly fixed, while lower level parameters are subject to modest evolution. Live parameters, continuously maintained and under configuration change control, are publicly available on-line [81].

The optimum frequency for the accelerating structures is determined by a number of factors. Lower frequencies are favoured due to looser tolerances in manufacturing cavity components. Lower frequencies also have the advantage of reducing Radio Frequency (RF) losses in superconducting cavities, decreasing beam losses through larger apertures, and ameliorating Higher Order Mode (HOM) effects [83] from the high current beams. Higher frequencies are encouraged by the desire to keep the size of the superconducting cavities small, making them easier to handle and reducing manufacturing costs. The cryogenic envelope and power consumption are also reduced at higher frequencies. Generally it is agreed that a frequency of 600–800 MHz is a good compromise for elliptical structures [84, 85].

The 4% duty factor of the long pulse beam structure is imposed using modulators to drive the klystrons. Special care has to be taken with the design of the RF power source, distribution system and controls, due to severe space limitations, reliability, safety concerns, high investment and operational costs. The baseline design is for one modulator and one klystron per cavity, giving maximum flexibility for beam tuning and robustness against faults. First studies show that the linac will – after retuning – be capable of operating with any single individual superconducting cavity off-line.

In the current design of the superconducting linac, acceleration fields or beam energy gained per cavity are limited by the surface electric fields in the cavities, rather than by the power that can be delivered through

Parameter	Unit	Value
Ion source output energy	MeV	0.075
RFQ output energy	MeV	3
DTL output energy	MeV	50
Spoke resonator output energy	MeV	191
Elliptical medium beta output energy	MeV	653
Elliptical high beta output energy	MeV	2500
Proton kinetic energy on target	MeV	2500
Ion source length	m	2.5
LEBT length	m	2.1
RFQ length	m	4.9
MEBT length	m	1.2
DTL length	m	19.0
Spoke resonator section length	m	75.0
Elliptical medium beta section length	m	117.0
Elliptical high beta section length	m	200.0
HEBT length	m	163.3
Linac + HEBT Length	m	582.5
Depth of linac below ground level	m	10
Number of accelerating gaps per spoke cavity		3
Number of cells per medium beta cavity		5
Number of cells per high beta cavity		5
Spoke resonator cavities per cryomodule		2
Medium beta elliptical cavities per cryomodule		4
High beta elliptical cavities per cryomodule		8
Optimal beta, spoke resonators		0.50
Geometric beta, medium beta elliptical cavities		0.70
Geometric beta, high beta elliptical cavities		0.92
Operational gradient, spoke resonators	MV/m	8
Operational gradient, medium beta cavities	MV/m	15.44
Operational gradient, high beta cavities	MV/m	18.17
Maximum power transmitted to beam, High beta cavities	мŴ	0.9
Number of modules in spoke section		18
Number of modules in medium beta section		16
Number of modules in high beta section		14
Cavities per spoke cryomodule		2
Cavities per medium beta cryomodule		4
Cavities per high beta cryomodule		8
Quadrupoles per spoke cryomodule		2
Quadrupoles per medium beta cryomodule		2
Quadrupoles per high beta cryomodule		2

Table 20: Lattice and Accelerator Science parameters, December 16, 2011. The HS_2011_11_23 lattice is optimised for 50 mA operation, with a single cavity and a single modulator per klystron, and hybrid cryomodules.



Figure 59: The power gained by a 50 mA beam in each of the cavities of the HS_2011_11_23 lattice [82]. The different background colours indicate different cavity types and an example of different power classes for the RF sources.

the power couplers. Figure 59 shows the power requirement for the RF sources, based on beam dynamics requirements for a smooth acceleration transition between the different types of structures. The variations within the cavity families are due to varying transit-time factors as the particle velocity changes, and to the requirement that the longitudinal focusing force changes smoothly between the different cavity families. The frequency doubling and consequent change of synchronous phase after the spoke resonator section mean that the power per cavity drops by approximately a factor of four, in order to maintain a constant longitudinal focusing force across that boundary.

The goal of being a sustainable research facility requires power consumption minimisation, and the re-use of all cooling water heat. The facility is divided into different categories depending on the cooling needs and the temperature range required for each set of equipment to operate reliably. Experience from SNS confirms that the highest temperature zones are the RF loads, circulators, compressors, and the klystron collectors. These hot systems enable the ESS to deliver commercially viable water – hotter than 70 C – for re-sale to the regional district heating system.

4.2 Beam physics

The goal of the beam physics studies for ESS is to achieve the top-level parameters listed in Table 2 with a design that is optimal in the sense that it minimises entities like cost, footprint on the site, energy consumption, beam losses and radio-activation, and maximises others like reliability, flexibility and upgradeability. To reach this goal, a linac has been chosen consisting of a proton source, a magnetic LEBT, an RFQ, a MEBT, a DTL, a section of spoke resonators, sections of medium beta and high beta elliptical cavities and the HEBT which includes room for an energy upgrade and a system that delivers the beam to the spallation target [86].

The choice of parameters and layout reflects the state of the art of accelerator and neutron science. Advances in superconducting radio frequency technology since the ESS design of 2002/2004 [3, 4] have led to an increase in beam energy and a decrease in beam current, since radio frequency cavities have become relatively less costly and more reliable compared to the handling of very high beam currents. Similarly, progress in neutron science has made the production of short neutron pulses, requiring H⁻ ions and an accumulation ring, less motivated. Thus the ring has been abandoned and protons are used instead of H⁻. In spite of these developments, it is still a daunting beam-physics challenge to design a linac that can accelerate the 5 MW beam with sufficiently low losses and high reliability. Part of this challenge is to find methods that allow the prediction of critical performance factors, such as beam losses, with sufficient accuracy.

4.2.1 Design, optimisation and beam dynamics

There are potentially many different tools available both for the design of the linac and to study the evolution of the beam through the linac, verifying the design. Beam-dynamics calculations for the ESS linac have so far been made using the CEA suite of codes with Toutatis for the RFQ, GenLinWin for the design of the superconducting linac and TraceWin for particle tracing. These will be complemented by other codes in the future.

Ion source. The ion source, described in the section about the warm linac, and its output beam properties are the input to the beam-dynamics calculations for the accelerator. In this respect, the most important source parameter is the beam emittance, or more generally, the phase-space distribution of the proton beam at the exit of the source. Also important are temporal characteristics such as beam stability over a wide range of time scales. The beam energy is 75 keV as given by the ion-source platform. For the purpose of the beam-dynamics calculations presented here, the beam is DC. The phase space distribution of the beam at the exit of the ion source is complex. Nonetheless, pending the availability of a more realistic particle distribution out of the LEBT, it is assumed that the beam at the RFQ input is a 4D waterbag distribution with a normalised RMS emittance of 0.20 π mm mrad.

LEBT and RFQ. The Low Energy Beam Transport transports the beam from the exit of the ion source using two solenoid magnets to provide a tight focus at the entrance of the Radio Frequency Quadrupole (RFQ). To avoid emittance blow-up due to the strong space-charge forces at the low energy of 75 keV, the beam in the LEBT will be space-charge neutralised by electrons produced either by the beam itself in interactions with the residual gas or through injection of free electrons into the beam. The LEBT is also expected to include a chopper which gives the beam pulse sharp rising and falling edges, avoiding transient beam loss while, for example, the ion source current stabilises or the RFQ field reaches its full value.

The RFQ [87] bunches the beam at 352.21 MHz and accelerates it to 3 MeV while simultaneously focusing it transversely. It is optimised for minimum beam loss and the best possible beam quality at its output. It is designed for 100 mA beam current in order to provide a high reliability at the initial beam current of 50 mA but also as a preparation for future power upgrades of ESS. Figure 60 shows the results of beam-dynamics simulations of the RFQ using TraceWin. The transverse emittances (red and blue curves) are conserved throughout the RFQ, while the longitudinal emittance reaches 0.25 π mm mrad at the end of the RFQ.

The distribution and behaviour of the outermost particles in the beam halo are also important, in addition to the emittances of the beam. Figure 61 shows the particle density along the RFQ, resulting from the tracking of 50,000 macro-particles. It is seen that the beam at the exit of the RFQ is confined within a radius of 3 mm. The transmission is 100% for beam currents up to at least 75 mA, decreasing to 99% at 100 mA.

MEBT and DTL. The Medium Energy Beam Transport is not designed yet, although a zeroth order lattice exists. It can even be discussed whether a MEBT is needed. It inevitably causes some emittance and halo growth with its relatively weak focusing between the strongly focusing RFQ and Drift Tube Linac structures. Reasons to nevertheless have a MEBT a few metres long would be to create room for a chopper that is faster than the one in the LEBT, if this would be needed, for beam instrumentation, scraping and collimation, as well as to give the possibility to steer the beam and adjust Twiss parameters from the RFQ into the DTL.



Figure 60: Emittance through the RFQ in horizontal (red), vertical (blue) and longitudinal (green) planes.



Figure 61: Radial particle density distribution as a function of radius and distance along the RFQ.

The ESS DTL is expected to be similar to that of Linac4 at CERN, and it will consist of three separate tanks operating at 352.21 MHz. The lattice structure of the DTL is not yet fixed although a FODO structure is preferred at present, and this is what is used for the end-to-end simulations shown below.

Superconducting Linac. In the design of the superconducting linac with its three families of cavities – spoke resonators and elliptical cavities of two different geometrical betas ("medium" and "high") – 11 parameters have been considered as free, and their values have been optimised to achieve the shortest possible linac. Although there are many other design goals than a short linac, it can be argued that several of those correlate positively with a short linac. These include the number of cavities, RF sources and cryomodules, and thereby static cryogenic loads, power consumption, reliability and maintainability. The length thus should correlate positively both with performance and cost of the facility.

The 11 free parameters are the geometric betas of the 3 cavity families, the 2 transition energies where one family changes to the next, the number of cells per cavity (3), and the number of cavities per cryomodule (3). Constraints in the optimisation are, apart from the final energy, the maximum fields in the cavities, maximum power delivered to the beam through each power coupler, rules of thumb in linac design concerning the synchronous phase, transverse and longitudinal betatron phase advances and their derivatives, and mechanical dimensions of components that make up the linac. The sensitivity to variations around the optimum for some of the parameters is small, and in these cases layouts with a smaller number of cavities or cryomodules are chosen.

4.2.2 End-to-end lattice and simulations

The current design layout and optics, HS_2011_11_23, has the main parameters listed in Table 20. This design is based on the so-called hybrid concept for the cryomodules, where these are built as separate cryostats, but where the space between the cryostats is enclosed by an interconnecting sleeve cooled to an intermediate temperature such as the 70 K of the outer thermal screen of the cryostats.



Figure 62: Horizontal, vertical and longitudinal beam sizes in the HS_2011_11_23 lattice, from the entrance to the RFQ to the end of the last elliptical cavity. These are the RMS sizes of an initial 0.20 π mm mrad 4D waterbag distribution propagated through the linac without space charge.

Figure 62 shows the transverse and longitudinal beam size along the ESS linac, from the entrance of the RFQ to the end of the last accelerating cavity. This is the RMS size of a beam that initially has an emittance of 0.20 π mm mrad in a waterbag distribution, propagated through the linac without space charge. It is thus proportional to the square root of the beta functions. The average transverse beam sizes are approximately constant, indicating good matching of the Twiss parameters. The longitudinal size also has a smooth variation. Adding space charge, the density profile along the linac can be calculated through multi-particle tracking. The result with 100,000 particles is shown in Figure 63, with the black contour indicating the transverse acceptance. The RMS radius is similar to that in Figure 62, but not identical since space charge changes the focusing, and the outermost particle trajectories extend to about 8 times the RMS beam size.

Figure 64 shows the emittance growth along the linac, derived from the same tracking as in Figure 63. Most of the transverse emittance growth occurs immediately after the transitions from one structure to the next at the beginning of the linac, from RFQ to MEBT, from MEBT to DTL, and from DTL to the spokes section, where the focusing strength changes. Some longitudinal emittance growth also occurs in these locations. Overall, the emittance growth is small, and at the end of the linac, the emittance is 0.25π mm mrad in the two transverse



Figure 63: Transverse particle density distribution along the HS_2011_11_23 linac, with the black contour representing the clear aperture.



Figure 64: Horizontal (red), vertical (blue) and longitudinal (green) RMS emittance in the HS_2011_11_23 linac, from the entrance to the RFQ to the end of the last elliptical cavity.

planes, and 0.32 π mm mrad longitudinally.

The beam is expanded by a large factor at the end of the accelerator, onto the target window. More important than emittance growth is thus that the beam envelope, including halo, fits inside the acceptance of the machine in all three planes. This is true with a wide margin for an ideal machine – that is, one without misalignments of magnets or cavities, ripple and jitter on the RF, et cetera – the only case analysed so far. As an example, the longitudinal acceptance is illustrated by Figure 65, where the longitudinal phase space (energy vs. phase) occupied by a matched beam at the entrance of the superconducting linac is shown as the multicoloured ellipse. The blue background is the acceptance such that particles launched from anywhere inside that phase-space volume are transmitted through the entire linac.



Figure 65: Acceptance (blue background) and matched beam (multi-coloured ellipse) at the entrance to the HS_2011_06_22 superconducting linac.

4.2.3 Errors and tolerances

Calculations in the previous section were made with an ideal linac. In a real machine, finite precision and stability have to be considered, and the influence of errors on the linac performance has to be evaluated. The effects of errors also set specifications and tolerances on accelerator components. Errors can be static, such that they can be corrected or compensated for off-line, or they can be dynamic, in which case the accelerator design must be sufficiently forgiving to accommodate them.

Examples of static errors are misalignments of magnets and cavities, poor cavity performance requiring some cavities to be fed with less than nominal power and magnet imperfections including higher multipole components of quadrupole magnets. Dynamic errors include ripple or other instabilities in power converters, fluctuations in beam current, as well as amplitude variations and phase jitter of the RF systems. In an intermediate category belongs malfunctioning equipment, where work-arounds in some cases will be possible if schemes for re-tuning the linac are prepared and available on-line in the control room. Higher-order modes (HOMs) in the acceleration cavities may also be important for beam dynamics. These can be investigated and mapped in the construction phase, but their excitation depends on the beam. The sensitivity of the beam to HOMs must be studied, and the result may influence the design of the cavities.

Given the large number of RF power sources and their expected mean times between failures, it is highly desirable for the linac to be able to operate with at least one cavity out of order, for example due to a failed klystron. The early part of the linac is the most sensitive in this respect since the relative energy gain per cavity is larger there, and because any resulting mismatch or emittance growth will propagate through and affect all the remaining linac. Thus, a study has been made of cavity failures in the spokes section. Figure 66 illustrates the energy gain in the spoke cavities and which four specific cavities that were investigated: the first two, cavity number 23 where the particle energy gain is highest, and cavity number 28 which is the last one in

the spokes section. The first and the last cavity in the section are particularly critical, since they are used for the longitudinal matching to the neighbouring sections.

The conclusion of the study is that the failure of any single cavity can be handled after a local re-tuning of the amplitude of the neighbouring cavities plus re-adjustment of the phases of the downstream cavities due to a reduced beam energy. Some emittance increase is unavoidable, but it was limited to 25% in the worst case. Operation is also possible with a simultaneous failure of the first two cavities, but this requires that the phases of all the downstream cavities are readjusted, as well as the transverse matching between the linac sections.



Figure 66: Energy gain of particles through the spoke cavities of the HS_2011_06_22 lattice. The effect of cavity failure was studied for cavity numbers 1, 2, 23 and 28.



Figure 67: Particles falling out of the RF bucket in the superconducting linac and eventually getting lost in a case of unrealistically large RF amplitude ripple and phase jitter of 2% and 2 degrees.

4.2.4 Beam loss and collimation

Beam losses are intimately connected to errors and tolerances. All structures downstream of the RFQ have a sufficient acceptance so that the entire beam distribution is transmitted through an ideal linac. For the longitudinal plane, this is illustrated by Figure 65. Beam losses appear only when errors and a realistic particle distribution are introduced into the simulations. An example is seen in Figure 67, where particles falling out of the RF bucket are shown for a linac with a large RF amplitude variation and phase jitter. Particles outside the RF bucket will not be accelerated and will be lost before reaching the target since their energies will not be matched to the fields in focusing or bending magnets.

The widely accepted number for maximum acceptable beam loss is expressed as a maximum linear loss of beam power equal to 1 W/m. If the losses are higher, radio-activation may prevent effective maintenance in the linac tunnel, and less than 1 W/m is desirable in order to reduce the exposure of the staff to radiation. Realistic beam simulations that can accurately resolve such low losses in a 5 MW beam are challenging. They require a good statistical accuracy all the way out in the tails of the particle distribution, that all non-linear fields are included to sufficiently high order, that all physical processes are included (which, for instance, has so far not

been the case concerning charge-changing collisions between beam particles in H^- linacs), and that the machine and its errors are known with high precision. Furthermore, it is necessary to know the initial conditions with high accuracy, that is, the particle distribution in all six phase-space dimensions at the entrance to the linac.

Probably the only way to make sure that simulation results can be transferred to reality is to impose the initial conditions by scraping and collimating the beam early in the linac, and this scraping and collimation is one of the main tasks of the MEBT.

A further way to reduce the activation of linac components is to concentrate the beam loss to specific points by installing additional collimators there together with appropriate extra shielding. At these points, the collimators would remove the outermost particles, so that the remaining ones can stay clear of machine apertures and propagate to the next collimator or to the target without further losses. The most suitable locations for these collimators need to be investigated through beam simulations.

4.3 Normal conducting linac

The normal conducting linac of the ESS consists of a proton ion source, LEBT, RFQ, MEBT and DTL. The major challenge for this part of the accelerator is the preparation of a beam with a well-defined pulse (and macro-pulse) shape, a small emittance and minimal halo. This will minimise beam losses throughout the high energy part of the linac, while maximising the overall reliability of the ESS. The integrated design of this part of the linac is key, requiring the solution of a series of specific problems of accelerator physics, particularly because of strong space charge effects.

4.3.1 Ion source and Low Energy Beam Transport

Figure 68 shows the schematic layout of the ion source and the LEBT. Nominal ion source parameters are listed in Table 21. The high current proton source will be based on the know-how acquired during the design phase and the construction phase and the commissioning of the sources named TRIPS and VIS at INFN-LNS [88, 89] and of the SILHI source at CEA-Saclay [90], but some remarkable improvements are to be developed because of the high current needed at a lower extraction voltage and because of the timing structure requested from the RFQ which needs the inclusion of a fast chopper together with its beam dump. A proton current of 60 mA at 75 keV with a normalised emittance of 0.2π mm mrad is a challenge and a suitable extraction system operating at 75 kV has to be developed. A new design of the magnetic field profile is considered as essential and the microwave injection system will be deeply revised according to the recent experience gained with the VIS source. Additional improvements to be considered to increase the beam brightness are, electron enrichments investigations with passive methods (under way at INFN-LNS), and tests of new plasma heating methods with electrostatic Bernstein waves.



Figure 68: Schematic layout of the ion source and the Low Energy Beam Transport.

Parameter	Unit	Value
Peak current	mA	60
Energy	MeV	0.075
Length	m	2.5
Transversal emittance	$\pi~{\rm mm}~{\rm mrad}$	0.2
Longitudinal emittance	$\deg MeV$	0.2

Table 21: Ion source parameters, December 16, 2011.

Ion source emittance. A campaign of measurements with an emittance measurement device proved also the possibility to reach the stringent goal of emittance requirements, as described in Figure 69. The emittance for different magnetic field is given, showing that the rms emittance increases slightly with the microwave power, because for higher current stronger space charge effects occur. In general the ϵ_{rms} , measured for different permanent magnet configurations, is lower than 0.2π mm mrad. The measurements recorded in Table 22 confirm that the SILHI source, in pulsed mode operation at 90 mA, fulfills ESS requirements. Beam formation is almost independent of the repetition rate. The emittances of pulses with a duration of 3 ms at a repetition rate between 10 and 20 Hz are smaller than the required values. These achievements are obtained for a low power beam of about 7.5 kW. Optimum matching with the RFQ must be guaranteed for weeks.



Figure 69: Measured ion source emittances for different values of microwave power and magnetic field.

Rep. rate	Pulse length [ms]								
[Hz]	10	10 5 3 2.5 2.0 1.5 1.							
10	0.166	0.156	0.152	0.152	0.156	0.148	0.145		
20		0.162	0.152	0.153	0.144	0.143	0.116		
30		0.144	0.144	0.142	0.142	0.138	0.130		
40		0.148	0.148	0.142	0.134	0.129	0.146		

Table 22: Measured SILHI ion source emittances [π mm mrad] for different pulse lengths and repetition rates at a beam current of 90 mA, conforming with ESS requirements.

Slow chopper. The interface between the LEBT and the RFQ takes into account different, competitive, requirements. The LEBT is at the right end of Figure 68, with parameters in Table 23. It is as short as possible, but contains beam diagnostics and a slow chopper, which ensures that the beam injected into the RFQ has a maximum rise and fall time of 100 ns, despite ion source rise and fall times between 50 μ s and 100 μ s. A slow chopper with similar characteristics has already been developed for the SPIRAL 2 project, using technology that is directly applicable to the ESS.

Parameter	Unit	Value
Length	m	1.6
Transverse acceptance	π mm mrad	0.4
Longitudinal acceptance	$\deg MeV$	0.3
Vacuum	mbar	10^{-5}
Focusing type		2 solenoids

Table 23: Low Energy Beam Transport parameters, December 16, 2011.

4.3.2 Radio Frequency Quadrupole

The local parameters of the reference design of the 4-vane RFQ evolve as a function of distance as shown in Figure 70, while Table 24 lists the global parameters. The RFQ accelerates a proton beam from 75 keV to 3 MeV, while focusing and shaping the beam into a train of bunches suitable for subsequent acceleration in the rest of the linac. Emittance and transmission results from the simulation code Toutatis [91] for 50 mA and 75 mA beam currents are shown in Table 25. The RFQ is predicted to deliver high quality beams with a total transmission of greater than 99% for nominal 50 mA beam currents. Negligible transverse emittance growth is observed for uniform and gaussian distributions (truncated at 4σ), in all cases with an input transverse RMS emittance of 0.2 π mm mrad.



Figure 70: Reference design parameters as a function of distance along the RFQ.

Parameter	Unit	Value
Output energy	MeV	3.0
Length	m	4.95
RF frequency	MHz	352.21
Temperature	Κ	300
Axial Electric Field, E_0 , max	MV/m	2.123
Peak electric field on poles	Kilpatricks	1.8
Pole radius R_0 , minimum	mm	3.445
Pole radius R_0 , average	mm	4.091
Pole radius R_0 , maximum	mm	4.737
Minimum aperture a , minimum	mm	2.972
Minimum aperture a	mm	3.482
Minimum aperture a , maximum	mm	3.932
Intervane voltage, minimum	kV	80
Intervane voltage, maximum	kV	120
Vane tip radius of curvature, ρ	mm	3
Total length of vanes	m	4.92
Modulation factor, maximum		2.04

Table 24: Radio Frequency Quadrupole parameters, December 14, 2011.

Current	Distribution	Output RM	Transmission	
[mA]		Transverse $[\pi \text{ mm mrad}]$	$ Longitudinal [\pi \text{ mm mrad}] $	[%]
50 50	Uniform Gaussian	$0.21 \\ 0.21$	$0.26 \\ 0.28$	99.40 99.56
75 75	Uniform Gaussian	$0.21 \\ 0.20$	$\begin{array}{c} 0.30\\ 0.32 \end{array}$	98.98 98.66

Table 25: Simulated RFQ output emittance and transmission, for 2 beam currents and 2 beam distributions.

4.3.3 Medium Energy Beam Transport

Figure 71 shows the four quadrupoles that match the beam characteristics transversely, and the two buncher cavities that match longitudinally, in the compact MEBT between the RFQ and the DTL. Table 26 lists the nominal parameters. The 3 main goals of the MEBT are to:

- 1. Collimate the beam halo, adjustable blades.
- 2. Measure the beam phase, emittance and profile.
- 3. Match the RFQ output to the DTL input both transversally and longitudinally.

A shorter MEBT has better beam dynamics performance, but a minimum distance between elements is required in order to fit vacuum flanges, diagnostics elements, et cetera. Emittance evolution through the MEBT is shown in Figure 72. The gradient of the 70 mm compact quadrupole ranges from 9 T/m to 33 T/m. It incorporates dipole steering to correct beam misalignments. Studies have been performed considering the potential inclusion of a fast chopper and its corresponding beam dump into the MEBT, although this is not a hard requirement, since there is no need for a charge injection scheme into an accumulator ring.

Buncher. The buncher design process iterates between electromagnetic, thermo-mechanical, RF, and beam dynamics issues that also affect tuner and coupler design.



Figure 71: Compact MEBT layout, with four quadrupoles and two buncher cavities.

Parameter	Unit	Value
Length	m	0.6
Number of RF bunchers		2
Number of quads		4
Acceptance	mm	20
Buncher parameters		
Buncher power, E_0TL	MV/m	0.5
Shunt impedance per unit length, ZT^2	$M\Omega/m$	8.344
Peak field	Kilpatrick	< 1.7
Surface peak field	MV/m	25.35
Quality factor, Q		$26,\!415$

Table 26: Medium Energy Beam Transport parameters, May 19, 2011



Figure 72: Left: Emittance growth through the MEBT in the horizontal (red), vertical (blue) and longitudinal (green) planes. Right: RMS beam size envelopes.

4.3.4 Drift Tube Linac

DTL Alvarez linacs have had a long and successful history. Recent designs (as at the SNS and LINAC4) are characterised by high frequency structures, permanent magnets and high duty cycle operation. Permanent magnet quadrupoles allow an improvement of shunt impedance (with smaller drift tubes) and substantial simplification of cabling and logistics. The reduction of the number of components is a clear advantage for the reliability and availability of the accelerator. The present design foresees 3 tanks as described in Table 27. The tank length is determined by the available RF power. The main parameters are shown as a function of distance along the DTL in Figure 73. Since every tank transition is a source of potential beam mismatching and quality degradation, the first tank is closed at a relatively high energy. The maximum surface field is limited to $1.4 E_{kp}$ (Kilpatrick field) along the structure, and to $1.2 E_{kp}$ in the first cells due to the presence of the quad magnetic field (Moretti criterion).

The nominal focusing scheme uses a FODO lattice with a focusing period of $4\beta l$. Empty drift tubes contain beam position monitors and dipole steering magnets. The maximum gradient in the 62 permanent magnet quadrupoles is about 75 T/m. With this scheme it is possible to correct misalignment errors for realistic tolerances consistent with careful emittance preservation and very low beam losses. The mechanical design, based on the LINAC4 design, allows accurate positioning and alignment of tube position using all metallic gaskets. A prototype tank was built a few years ago in a collaboration between CERN and INFN. The maximum length for a mechanical module is about 2 m. The tank is stiff enough to be assembled off-line and then transported into the tunnel. The 8 m long tank will probably be one of the largest elements of the linac to be installed. The RF power is delivered to the cavity via two couplers with planar windows and lateral wave guide slots following CERN design. Slow tuning will be achieved with movable plungers.

Parameter	Unit	Value
Output energy	MeV	50.0
Length	m	19.0
RF frequency	MHz	352.21
Temperature	Κ	300
Accelerating gradient	MV/m	3.0
Number of tanks		3
Number of RF power sources		3
Power per RF power source	MW	2.5
Power at coupler	MW	1.0
Mechanical length of module	m	2.0

Table 27: Drift Tube Linac parameters, November 14, 2011.



Figure 73: Main parameters as a function of distance along the Drift Tube Linac.

4.4 Spoke resonator cavities

The superconducting spoke section of the linac accelerates beam from the normal conducting section to the first family of the elliptical superconducting cavities. As indicated in Table 28, acceleration will be performed by a single family of bulk niobium spoke cavities. A total of 36 spoke cavities, grouped by 2 in 18 cryomodules, fill 75 m of spoke linac length. The chosen operating accelerating field is 8 MV/m – where the accelerating length is defined to be $(n + 1)\beta\lambda/2$, and n is the number of spoke bars. This corresponds to a peak field E_{pk} of 40 MV/m. These values are chosen to take into account the actual state of the art in performances limitations for medium beta SRF cavities due to field emission. The required peak RF power to supply the cavity is about 250 kW for the 50 mA beam intensity, corresponding to 10 kW of average power. As Table 29 records, only about 15 spoke prototypes of different types and β 's have been fabricated and tested worldwide. However, other high power proton accelerators currently under design are also considering whether to adopt spoke technology: MYRRHA in Belgium, ADS in China, Project-X in the USA and EURISOL in Europe. The ESS linac will probably be the first to be constructed with spoke cavities.

The choice of spoke resonator structures is driven by the potential for high performance, and intrinsic mechanical advantages. In addition to the well known advantages of superconducting cavities – high efficiency, large beam aperture, and high reliability – spoke cavities also:

- have multi-gap capabilities (high real-estate gradients)
- are compact and naturally stiff (less sensitive to mechanical perturbation such as vibrations)
- exhibit high cell to cell coupling (no field flatness required)
- are less sensitive to HOM or trapped modes (due to the high cell to cell coupling)
- are not submitted to dipole steering effect (contrary to other medium beta cavities like quarter-wave resonators)
- have a wide β range accessible
- exhibit a high longitudinal acceptance (accelerating efficiency over a wide β range)

Parameter	\mathbf{Unit}	Value
Output energy	${ m MeV}$	~ 200
RF frequency	MHz	352.21
Temperature	Κ	2
Operational gradient	MV/m	8.5
Operational voltage	MV	3.3
Number of RF power sources		45
Power transmitted to the beam	$^{\rm kW}$	165
E_{peak}/E_{accel}		4.1
B_{peak}/E_{accel}	$\mathrm{mT/(MV/m)}$	9
Expected gradient, horizontal	MV/m	8.5
Expected gradient, vertical test	MV/m	10
Cavity quality factor Q_0 (low field)		$5 imes 10^9$
Niobium thickness (nominal)	mm	4
Beam port aperture	mm	50
Coupler port aperture	mm	56
Nominal power for FPC conditioning	$^{\rm kW}$	400
Cavity β		0.50
Cavity length	mm	687
Cavity diameter	$\mathbf{m}\mathbf{m}$	492

Table 28: Spoke resonator parameters, November 14, 2011.

4.4.1 Cavity design

Electromagnetic design. The spoke cavity EM Design is guided by the frequency, the optimum beta and then the optimisation of the peak fields. Whereas the most important parameter for the beam is the accelerating field or the voltage seen by the particle, the most important optimisation criteria is the ratio of surface fields to

Lab	Туре	Freq. [MHz]	Optimal β	$E_{acc} \max$ [MV/m]	V_{max} [MV]	E_{pk}/E_{acc}	$\frac{B_{pk}/E_{acc}}{[\text{mT}/(\text{MV/m})]}$
IPN Orsay	Single	352 352	0.20	4.8	0.8	6.7 4.7	14.5 12.8
	Single	302	0.30	0.1	2.0	4.7	12.0
ANL	Single	855	0.28	4.4	0.3	5.5	12.7
	Single	345	0.29	8.7	2.2	4.6	12.1
	Single	345	0.40	7.0	2.4	6.3	16.7
	Double	345	0.40	8.6	4.5	4.7	9.1
	Triple	345	0.50	7.6	6.6	3.7	11.5
	Triple	345	0.62	7.9	8.7	3.9	12.0
FZ-Juelich	Triple	760	0.20	8.6	1.4	5.1	13.3
LANL	Single	350	0.21	7.5	1.3	5.1	13.3
	Single	350	0.21	7.2	1.3	5.0	10.1
FNAL	Single	325	0.21	12.0	2.4	3.6	5.8
	Single	325	0.21	16.7	3.4	3.6	5.8
$at \ 2K$	Single	325		21			

Table 29: Worldwide performance of all spoke resonators at 4 K.



Figure 74: Optimisation of the spoke bar shape. Left: Elliptical. Right: racetrack.

peak fields, that is to minimise the peak fields keeping constant the accelerating field. Another important factor to optimise is the cavity overall length: a spoke cavity has a reentrant shape, and the size of the re-entrant part can be increased to give more volume to store the energy, thus resulting in a peak field decrease. Of course, the drawback is a lower real-estate gradient due to the higher longitudinal space taken by the cavity for the same voltage. In the process of peak field optimisation, the shape of the spoke bars is the most important factor. Previous work performed on a triple spoke cavity for EURISOL showed that racetrack shapes or elliptical shapes of the spoke bar close to the beam aperture could reduce the peak fields. This optimisation is illustrated in Figure 74. Special attention is being paid to the ease of spoke cavity fabrication, and dedicated features are being designed to facilitate the welding of difficult parts – for instance, the weld between the spoke bar base and the cavity body. Figure 75 shows the result of the conceptual design of the spoke cavity. Peak surface fields are located around the spoke bar, close to the cavity body for the magnetic field, and close to the spoke bar iris for the electric field, as shown in Figure 76. The distribution of the electric field is plotted in Figure 77.

Mechanical design and helium tank. The mechanical analysis of the spoke cavity consists in defining the thickness of the niobium walls and defining the required stiffeners to minimise the Lorentz forces detuning due the cavity high electromagnetic fields. The helium tank type and design is also an important aspect in the overall mechanical behaviour of the cavity. Mechanical calculations will be performed with niobium thickness ranging from 3 mm to 6 mm. Different stiffener designs will be investigated, located around the weakest part of the cavity – the re-entrant part around the beam tubes. Several materials and attachment points to the cavity for the helium tank will be considered, including stainless steel and titanium. Calculations already performed on a triple spoke cavity for the EURISOL project showed that 4 mm, hollowed disks for the stiffeners and titanium tank are interesting options for such cavities, as shown in Figure 78.

4.4.2 Cold tuning system

Requirements. The cold tuning system (CTS) is a device attached to the spoke cavities meant to adjust *in-situ* the resonant frequency of the superconducting cavities in order to counteract frequency shifts due to



Figure 75: Overall aspect of the double spoke cavity.



Figure 76: Distribution of surface fields in the spoke cavity. Left: Electric. Right: Magnetic.



Figure 77: Electrical field along the cavity beam axis ($L_{acc} = 780 \text{ mm}$).



Figure 78: View of the EURISOL triple spoke tank and stiffeners.

mechanical perturbations of the cavities. For a pulsed machine like ESS, the Lorentz force detuning is another important source of resonant frequency detuning and its effect should be carefully taken into account. The spoke CTS should integrate two different functions: a slow tuning capability over a wide frequency range (typically 1 MHz) and a fast tuning capability over a reduced frequency range (a few kHz). The first function is provided by a mechanical system driven by a stepping motor, and the second function is obtained by means of piezoelectric actuators inserted in the mechanical system of the CTS.

Design. Two alternatives for the cold tuning system are being developed in parallel. This first system is based on the mechanical deformation of the cavity by either pulling or pressing on the cavity extremities in order to change the cavity length, thus resulting in a frequency detuning. The second solution is based on a niobium plunger inserted in the cavity to change the cavity volume and thus changing its resonant frequency. The second solution, quite standard for room temperature RF devices is quite innovative for SC cavities, as pollution problems may arise from the displacement of an object inside the cavity volume.

The CTS consists of a mechanical system (Figure 79) driven by a cold stepping motor operating under vacuum and a moto-reductor. The motor drives a ball screw, linked to a double lever arm mechanism which can act on four rods attached to the cavity. The design is optimised to obtain high rigidity, lowest possible weight and cost. The alternative solution base on a niobium plunger will be derived from the technical solutions developed by IPN Orsay for the Spiral-2 quarter-wave resonators. The final choice will be made on the performance and reliability analysis of both solutions.



Figure 79: Cold tuning system for spoke resonators.

4.4.3 Power couplers

Requirements. The power coupler has the double role of supplying RF power to the cavity while insulating the cavity vacuum from the atmospheric pressure inside the RF line. For the ESS double spoke resonator, operated at 8 MV/m, the nominal power for the linac baseline (50 mA, 4% duty cycle) is about 250 kW peak power (10 kW average power). Several upgrade scenarios are being envisaged for the ESS linac. The most demanding one in terms of additional requirements for the power coupler is the beam current increase to 75 mA. In that configuration, the corresponding RF power requirement is close to 400 kW.

Conceptual design. A pre-analysis of the possible solutions for the spoke RF coupler has been performed based on recent developments for the EURISOL project. A capacitive 352 MHz power coupler has been developed for spoke cavities, to be mounted on a 56 mm diameter port. To take into account the high peak power requirements and to cope with the increased capability required for the potential upgrade, an adaptation to a larger coupler diameter will be done. The coupler geometry is coaxial, at 50 Ω , using a warm disk ceramic window. Two pipes located on the window outer diameter give the possibility to water-cool the ceramic (Figure 80). Several window geometries have been studied: cylindrical, disk (with and without chokes) and travelling wave window. For each window type, the HFSS software was used to calculate the RF parameters, the surface field on the ceramics, the bandwidth, and the RF losses. Finally, the design based on a disk ceramic without choke was chosen because it was the best compromise between good RF performances and simplicity, leading to a reliable and cost-effective design. A computed S_{11} parameter of -57 dB is obtained at the nominal frequency. The coupler exhibits a very large bandwidth, thereby allowing standard fabrication tolerances.



Figure 80: Conceptual design of a 352 MHz spoke power coupler of 56 mm diameter and computed return loss S_{11} .

4.5 Elliptical superconducting cavities

The elliptical superconducting linac consists of two types of cavities – medium beta and high beta – to accelerate the beam from the spoke superconducting linac up to full energy. The profile of a 5-cell high beta cavity is shown in Figure 81, while the main RF cavity parameters are listed in Table 30. The linac layout optimisation has been carried out taking into account the limitations of SRF cavity performance, that is field emission. This is reflected in the choice of the parameters such as the maximum accelerating gradient E_{acc} , and the peak electric field on the surface E_{pk} . The power couplers run derated, ensuring that it is possible to add a 30% power margin for cavity voltage stabilisation.



Figure 81: Geometry of the prototype high beta ($\beta = 0.86$) cavity.

4.5.1 Cavity design

Cavity requirements. The elliptical cavity parameters have been chosen taking into account the state of the art performance of bulk Nb cavities but also the actual performance of cavities in operating linacs, reflecting the commonly observed online performance yield which differs from the single cavity vertical tests.

The maximum E_{pk} specification is linked to the expected performance regarding field emission (FE) in elliptical cavities. High pressure water rinsing (HPWR) has proven to be the most efficient processing step to push the FE onset to sufficiently high gradient that it is not the main performance limiting factor. Currently the largest available set of multi-cell high gradient cavities consists of 9-cell 1.3 GHz Tesla/XFEL-type cavity. Using state of the art preparation and cleaning techniques several laboratories have proven that accelerating gradients at the XFEL specifications ($E_{acc} = 23.6$ MV/m, corresponding to $E_{pk} = 47$ MV/m, and $B_{pk} = 100$ mT) can be obtained on series production. More interesting is the usable gradient yield statistics from a production run of 50 cavities [92] showing that a 20 MV/m gradient (corresponding to 40 MV/m peak surface electric field) is obtained for about 80 to 90% of the cavities. In most cases, field emission limited cavities can be re-processed with extra steps of HPWR with 80% success rate. The ESS elliptical cavity peak field specifications are reduced by about 20% with respect to XFEL ones to ensure a high performance yield despite the larger cavity size and reduced betas.

High beta prototype cavity design. One of the main parameters in the design of a multi-cell cavity is the cell-to-cell coupling κ . Choosing a low κ value emphasises the cavity efficiency only. With increasing κ , the efficiency is reduced but major gains numerous: it is easier to achieve an even field distribution in the cavity, and therefore to control the homogeneity of the peak surface fields among the cells. The frequency separation between the accelerating mode and its neighbour is also increased. Even more important for a high current application, the high κ translates into higher iris diameters, and better high order mode (HOM) propagation. We have investigated designs with different κ values from 1.1 to 2.5% for the $\beta = 0.86$ cavity. The conclusion was that the loss in cavity efficiency was excessive above $\kappa = 2\%$.

One important geometrical parameter for multi-cell elliptical cavity design is the wall angle. This is related to mechanical stability, sensitivity to Lorentz force detuning, and to the ease of cavity preparation (chemical etching, HPWR and drying) – a key activity in achieving high performance. A minimum wall angle of 8 degrees has been chosen, based on experience with $\beta = 0.5$ and $\beta = 0.65$ cavities [93, 94]. This choice necessarily restricts the range of geometrical cell parameters accessible for cavity optimisation for peak field performance.

Taking into account the cryogenic duty cycle, the average power dissipated in one cavity at 18 MV/m is less than 5.3 W at the Q_0 specification. The field distribution of the fundamental mode is shown in Figure 81 and the impedance of the fundamental passband modes is shown in Figure 82. Only the $4\pi/5$ mode has significant impedance in the energy range of the high beta section (β between 0.76 and 0.96), besides the accelerating mode. The $4\pi/5$ mode cannot be avoided in this type of cavity.

External coupling and end-groups. The matched Q_{ext} at the specified beam current and nominal gradient is 7.1×10^5 . The power coupler connection is a 100 mm, 50 Ω coaxial line. The nominal Q_{ext} value is achieved by combining a 140 mm beam pipe diameter and using a conical shape coupler tip with a penetration of 7 mm in the beam tube, as shown in Figure 83. One benefit of a large beam tube diameter is the reduction of the HOM cutoff frequency. The cavity has identical end cells with straight beam pipes to fully exploit this possibility.

Parameter	Unit	Value
RF frequency	MHz	704.42
Temperature	Κ	2
MEDIUM BETA PARAMETERS		
Output energy	MeV	654
Number of cells per cavity		5
Geometric beta		0.7
Cavity length	m	1.145
Expected gradient, horizontal	MV/m	15
Expected gradient, vertical test	MV/m	17
Cavity Q_0	,	$6.0 imes 10^9$
Fundamental mode Q_{ext}		$6.8 imes 10^5$
Fundamental mode R/Q	Ω	340
Average heat load at nominal gradient	W	5.9
Power coupler power forward power	MW	1.2
Maximum Power transmitted to beam	MW	0.6
HIGH BETA PARAMETERS		
Output energy	MeV	2500
Number of cells per cavity		5
Geometric beta		0.9
Cavity length	m	1.356
Nominal gradient in the linac	MV/m	18
Expected gradient, vertical test	MV/m	20
Geometric beta prototype	,	0.86
Optimum beta		0.92
Cavity length prototype	m	1.315
Fundamental mode R/Q prototype	Ω	477
Fundamental mode Q_{ext} prototype		7.1×10^5
Cavity Q_0 at nominal gradient, prototype		6.0×10^9
Average heat load at nominal gradient, prototype	W	5.2
Power coupler power rating	MW	2
Power coupler forward power	MW	1.2
Maximum power transmitted to beam	MW	0.9
Cell to cell coupling	%	1.8
E_{pk}/E_{acc}		2.2
B_{pk}/E_{acc}	mT/(MV/m)	4.3
G	Ω	241
π and $4\pi/5$ mode separation	MHz	1.2
Iris diameter	$\mathbf{m}\mathbf{m}$	120

Table 30: Medium beta elliptical cavity and High beta elliptical cavity parameters, November 14, 2011.

Calculations of cavity high order modes have been made, focusing on the study of the TM monopole modes, since their excitation is more relevant than the excitation of dipole modes for the beam dynamics in a proton linac [95, 96]. The monopole modes have been computed using three different RF codes in 2D and 3D, with consistent results. Only two HOM monopole bands are below cutoff. The closest monopole HOM to a machine line is 12 MHz above it. The RF window of the power coupler, the doorknob waveguide transition and a length of rectangular wave guide are included in the EM simulations in order to take into account the full coupler transmission characteristics, and in order to assess the damping provided by the normal conducting parts of the power coupler and bellows located between cavities. The simulations indicate that the loaded Q's of the non-propagating monopole HOMs of a single cavity are all in the $10^4 - 7 \times 10^5$ range, thanks to the contribution of the normal conducting elements. The monopole HOM with the lowest frequency has the highest Q among monopole HOMs, due to its field distribution concentrated in the cell opposite to the power coupler port. This is illustrated in Figure 83.

4.5.2 Mechanical design

Since these cavities work in pulsed mode, it is important to minimise their sensitivity to Lorentz detuning. To this end stiffening rings are placed between the cavity cells. The static Lorentz coefficient, $K_L = \Delta f / E_{acc}^2$,



Figure 82: Impedance of the fundamental passband modes R/Q, as a function of β .



Figure 83: Elliptical cavity geometry and higher order mode performance. Left: Geometry of coupler-side end-group. Right: Lowest frequency TM monopole mode.

measures the resonance frequency shift produced by the mechanical deformation induced by the electromagnetic field in continuous wave operation. The positions of the stiffening rings and the cavity thickness have been optimised in order to minimise $|K_L|$ when the cavity has fixed extremities. The result is a cavity thickness of 3.6 mm and a stiffening ring radius of 84 mm. With these values, $|K_L| = 0.36 [\text{Hz}/(\text{MV/m})^2]$ for a cavity with fixed ends. A list of the corresponding RF and mechanical parameters is given in Table 31.

Parameter	Unit	Value
K_L fixed ends	$\mathrm{Hz}/(\mathrm{MV}/\mathrm{m})^2$	-0.36
K_L free ends	$\mathrm{Hz}/(\mathrm{MV/m})^2$	-8.9
Stiffness	$\rm kN/mm$	2.59
df/dz	m kHz/mm	197
Maximum VM stress versus elongation	MPa/mm	25
$K_P = df/dP$: fixed ends	Hz/mbar	4,85
$K_P = df/dP$: free ends	Hz/mbar	-150
Maximum VM stress versus pressure: fixed	MPa/bar	12
Maximum VM stress versus pressure: free	MPa/bar	15

Table 31: Mechanical characteristics of the cavity. The K_P parameters listed correspond to the elastic deformation that occurs when the cavity is operated in the cryomodule.

The static Lorentz detuning depends upon the external stiffness K_{ext} experienced by the cavity during operation, which is given by the tuner and helium tank combined stiffness. Taking into account the design stiffness of the tank and the measured stiffness of the Saclay V tuner [97], the expected $|K_L|$ is 1 [Hz/(MV/m)²].

The dynamic Lorentz detuning in pulsed operation will be compensated by a fast tuning system, using a Saclay V type piezo tuner, which has already been successfully used for Lorentz detuning compensation in pulsed mode with a $\beta = 0.5$ 704 MHz 5-cell cavity [97]. The helium vessel is made of titanium. The tuner is inserted between the cavity flange and the helium tank, as shown in Figure 84, and as in the SPL $\beta = 1$ cavity design [98]. The tank extends to the beam tube flange on the power coupler side and is stiffened with a series of fins. This layout enhances the ability to set the coupler port as close to the first cavity iris as needed, in order to achieve the correct coupling coefficient for the nominal beam power, and also for potential upgrades.



Figure 84: High beta elliptical cavity with a titanium helium vessel, and an integrated piezo tuner.

Before operation the cavity will be subjected to safety pressure tests at room temperature. Calculations of the plastic deformation expected in a 5 bar pressure cycle in a test rig indicate maximum residual deformations of less than 7 mm, which should not be detrimental to the field distribution of the fundamental mode. Two prototypes will be manufactured and tested in a vertical cryostat. They will be built from high purity bulk niobium sheet with a residual resistivity ratio (RRR) greater than 250. All flanges are made from niobium/titanium 45/55 alloy, directly weldable to niobium. The two prototypes will be equipped with two HOM 50 mm diameter ports.

Medium beta cavities. The medium beta cavities will share most of the mechanical features of the high beta cavities. The helium tank and tuner discussed above have already been adapted to a $\beta = 0.65$ 5-cell 704 MHz cavity at IPNO in the development of an SPL cavity prototype [99].

4.5.3 Fundamental power coupler

The RF power transferred through the coupler to the cavity is almost entirely converted into beam power, thanks to the very low dissipation in the SCRF cavity. The high beta elliptical cavity section running at the maximum gradient of 18 MV/m is the most demanding for power couplers, with the parameters shown in Table 32.

Parameter	Unit	Value
Nominal peak input power	kW	900
Maximum admissible input power	kW	1200
Maximum duty cycle	%	10

Table 32: Power coupler specifications.

Coaxial couplers using a single ceramic disk window are suited for handling both the peak and average power when equipped with active cooling. The 508 MHz KEK-B coupler type stands out as a very sound design for handling power levels of hundreds of kW in CW operation [100]. The KEK design has been adopted for the SNS power coupler specified at a peak power of 550 kW for a frequency of 805 MHz [101]. The SNS couplers have proven to operate reliably since the machine commissioning [102]. A coupler initially specified to handle 1 MW peak power at 704 MHz and 10% duty cycle has more recently been designed at Saclay following the same RF design principles, and after upgrading the inner conductor cooling. The prototypes shown in Figure 85 have been tested up to ESS parameters on a room temperature stand. Tests on a SCRF $\beta = 0.5$ cavity have also been carried out up to 1 MW in full reflection mode, the most demanding case for peak fields and power dissipation in the coupler [103]. It is foreseen to test a pair of these couplers up to 2 MW peak power, in order to evaluate the operational margins in terms of peak power.

The ESS coupler derives directly from this coupler design. The main differences lie in the mechanical interfaces with the cryomodule vessel, the reduced length of the air-side coaxial waveguide, and the cooling channels. Tests conducted in full reflection mode on a cavity using air cooling have been successfully carried out at up to 35 kW average RF power. The cooling channels will be modified to achieve a better efficiency, if air cooling is chosen over water cooling. The shorter air-side coaxial part already reduces the RF dissipation and improves the conductance of the channels for air flow.



Figure 85: Left: The CEA-Saclay 1 MW power coupler, with an outer diameter of 100 mm and an impedance of 50 Ω . Right: Scattering matrix coefficient S_{11} of the window, showing transmission characteristics with a very large bandwidth around the nominal frequency.

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air cooling is chosen over water cooling. The shorter air-side coaxial part already reduces the RF dissipation and improves the conductance of the channels for air flow.

RF window. The RF window is built around an alumina disk matched with chokes both on the inner and outer conductor. The connection between the RF window and the cavity is ensured by a stainless steel double walled tube which acts as the outer conductor of a coaxial line. The inner surface is deposited with copper to minimise the RF losses. The double wall encloses the He gas cooling channels necessary to cancel out the static losses to the 2K temperature of the coupler and to remove the heat produced by the RF dissipation in the copper layer.

Doorknob. The rectangular waveguide to coaxial transition uses the doorknob configuration. This most conveniently allows the interconnection of inner conductor cooling channels. It also allows a high voltage capacitor to be installed, necessary to apply a DC bias on the antenna in case a multipacting barrier coincides with the particular power level of a given cavity. The doorknob RF design reduces the peak electric field on the conductors in order to avoid discharges in air. The electric field distribution is shown in Figure 86. The maximum peak electric field at 1.2 MW RF input power is 12 kV/cm.



Figure 86: Electric field distribution in the doorknob transition between rectangular and coaxial waveguides.

4.6 Cryomodules

The end-to-end layout 2011_11_23 contains the cryomodules that are listed in Table 33. Fully equipped cryomodules (including cavities) provide an acceleration voltage for the beam. If superconducting quadrupole magnets are used, the cryomodules secondary function is to provide guidance for the beam. In order to fulfil these functions, an ESS cryomodule consists of a vacuum vessel cryostat, a number of superconducting accelerating cavities – connected to each other by bellows, two superconducting quadrupole magnets and associated equipment. The assembly of cavity packages is called the cavity string. The cryomodule provides an appropriate environment in which the internal components – namely cavities and magnets – can perform their main functions. The vacuum vessel of the cryomodule represents the interface with the outside. All external services are connected to the vacuum vessel. The conceptual layout of a cryomodule and its interfaces to outside services and equipment is shown in Figure 87.

Section	Number of modules	Module length Section length [m] [m]		Cavity count per module	Cavity count per section
High beta	14	13.812	200.368	8	112
Medium beta	16	6.800	116.800	4	64
Spoke	18	3.670	75.060	2	36
Utility slot	(47)	0.500			
TOTAL	48		391.728		212

Table 33: Cryomodule summary statistics.



Figure 87: Cryomodule component and interface schematic.

4.6.1 Cryomodule design

The associated equipment in and around the cryomodule includes main RF power couplers, High Order Mode couplers (HOM), tuners, RF cables, current leads for the quadrupole magnets, magnetic shielding, thermal shielding, cryogenic piping, helium bath heaters, vacuum pumps, other vacuum equipment (valves, gauges, connectors), beam instrumentation, cryomodule instrumentation, mechanical support systems and safety equipment. Cryomodules must enable:

• precise and accurate positioning and alignment of the active components with respect to each other and with respect to outside references

- cool down to and maintenance at the different cryogenic operating temperatures of the internal components, by removal of both static and dynamic heat loads
- thermal insulation of the internal components from the surroundings at ambient temperature in order to reduce static heat load
- adequate protection of the active components from vibrations
- protection of the entire module from overpressure
- protection of the active components from external magnetic fields
- a high degree of operational reliability

The nominal HS_2011_11_23 layout incorporates *hybrid* cryomodules. There are 2 other possible solutions which are still under consideration: *segmented* and *continuous*.

Hybrid

Basic design features. The hybrid cryomodule design consists of separate modules with an independent, external cryogenic distribution line, while using interconnecting sleeves between the modules to provide a) continuous cryogenic temperatures and b) an isolation vacuum even between cryomodules. A schematic representation of this concept is shown in Figure 88.



Figure 88: Schematic of hybrid cryomodule, with one cold gap (left), and one warm gap (right).

Advantages. The main advantages are (i) lack of the cold-warm transitions between cryomodules – reducing heat load significantly, (ii) the relatively easy transformation of any of the inter-module gaps from cold (as most of them will be) to warm, if required by beam instrumentation and (iii) the modularity, which allows extraction/replacement of any single cryomodule without affecting the whole string of cryomodules. A hybrid cryomodule section can be converted into a completely segmented machine by making all inter-module gaps warm.

Disadvantages. There are a number of open issues concerning the mechanical and thermal design of the hybrid cryomodule. The most important question to be answered is the actual heat load reduction to be achieved by the hybrid design. It should stand in relation to the added complexity and cost. The hybrid solution, like the continuous design, requires superconducting quadrupoles.

Segmented

Basic design features. Segmented cryomodules are independent cryostats that have their own insulation vacuum. They require an external cryogenic distribution line with jumper connections to each single cryomodule. An example is the SNS cryomodule shown in Figure 89.

Advantages. The major advantage of a segmented design is its flexibility. In case of preventive or corrective maintenance, there is no need to warm up a whole section of the accelerator – only the insulating vacuum of the affected cryomodule needs to be broken. All connections between cryomodules can be flanged, and only the jumper connection to the cryogenic transfer line needs to be cut and re-welded. (Bayonet connections can also be considered, to further increase flexibility.) This modularity keeps the MTTR low and reduces installation time. Another advantage is the possibility to place warm beam instrumentation – especially beam profile monitors, which are presently not available for operation at cryogenic temperatures – in any of the warm gaps between cryomodules.

Disadvantages. A segmented cryomodule has a higher heat load than continuous or hybrid cryomodules, because of the cold-warm transitions between modules. Their extra surface and the direct line of sight between



Figure 89: An example of a segmented cryomodule, from the SNS.



Figure 90: Examples of continuous cryomodules with internal cryogenic lines. Top: TESLA. Bottom: XFEL.

the 300 K beam pipe and the 2 K cavities translate directly to increased heat loads. Longitudinal space saving measures that simplify the heat intercept at the ends of the cryomodule can also induce additional heat loads. An external cryogenic transfer line also adds to the heat load.

Continuous

Basic design features. Several continuous cryomodules are connected to form a continuous cryogenic section for an adequate number of cavities. These sections are usually significantly longer than the length of a single cryomodule (which is limited to around 13 m by assembly and transport infrastructure). Cryogenic distribution lines are integrated into the continuous cryomodule, as illustrated in Figure 90, so that there is only one connection from the cryogenic system to the accelerator and jumper connections between the individual sections. There is one continuous insulation vacuum per section.

Advantages. A continuous integrated cryomodule has a reduced heat load, compared to segmented cryomodules, for two reasons: (i) there are no cold-warm transitions between cavity strings, eliminating the extra surface and the associated heat loads. Longitudinal space saving measures in segmented cryomodules can cause the simplification of the heat intercept at the ends of the cryomodule, inducing extra heat load. This effect is not present in a continuous design. (ii) integrating the cryogenic transfer line into the cryomodule increases the cryomodule diameter slightly but completely eliminates the need for an external cryogenic line. This reduces the total surface area of the cryomodule (plus transfer line), and therefore reduces the total heat load.

Disadvantages. The biggest disadvantage of a continuous design is its lack of flexibility. In case of preventive or corrective maintenance, the affected section of the accelerator must be warmed up entirely and its insulating vacuum must be broken. In the likely case that the internal connections between cryomodules are welded, there is always cutting and re-welding involved, both of which are important sources of contamination in the cryogenic lines. This complexity increases the MTTR. Another disadvantage is the exclusion of warm beam instrumentation. Some beam instrumentation devices – namely the beam profile monitors – are presently not available for operation at cryogenic temperatures. The use of warm beam instrumentation would dictate the interruption of the continuous cryomodule sections at a number of places, introducing warm sections for the placement of theses instruments. If there is no significant advance in development on cryogenic beam profile monitors, a fully continuous cryomodule design will not be feasible. The continuous design needs superconducting quadrupoles.

4.6.2 Elliptical cavity cryomodules

The most critical of the cryomodules is the high beta elliptical module. It has the highest number of cavities and it will be the first to be designed. One of the limiting parameters for the design of the high beta cryomodule is its total mechanical length, which is limited by two factors: (i) the length of the available clean room infrastructure, around 13.8 m, and (ii) the length of a 45-foot shipping container of 13.7 m. This limits the length of the cryomodule plus protective end caps to somewhat over 13 m. Any increases of the mechanical length of the high beta cryomodule would require rebuilding of the cleanroom infrastructure, which is a) very costly and b) not certain to be feasible, considering the existing building layout. Any increases of the transport length would induce complications and additional costs for the transport logistics. The present longitudinal layout of the high beta cryomodule is based on the 2011_11_23 cold linac layout. The lengths of components and distances between them are shown in Table 34. Figure 91 shows the realisation of these distances in a schematic view of the end of a high beta cryomodule slot.

The medium beta cryomodule will be a short variant of the high beta cryomodule. The present longitudinal layout of the medium beta cryomodule is based on the 2011_11_23 cold linac layout. The lengths of components and distances between them are shown in Table 34. Figure 91 shows the realisation of these distances in a schematic view of the end of a medium beta cryomodule slot.

Parameter	Unit	Value
HIGH BETA CRYOMODULES		
Length of cryomodule	$\mathbf{m}\mathbf{m}$	13820
End flange to quadrupole distance	$\mathbf{m}\mathbf{m}$	350
Quadrupole mechanical length	$\mathbf{m}\mathbf{m}$	410
Quadrupole to iris distance	$\mathbf{m}\mathbf{m}$	340
Cavity active length	$\mathbf{m}\mathbf{m}$	980
Iris to iris distance	$\mathbf{m}\mathbf{m}$	540
Centre to centre between cavities	$\mathbf{m}\mathbf{m}$	1520
MEDIUM BETA CRYOMODULES		
Length of cryomodule	$\mathbf{m}\mathbf{m}$	6800
End flange to quadrupole distance	$\mathbf{m}\mathbf{m}$	350
Quadrupole mechanical length	$\mathbf{m}\mathbf{m}$	410
Quadrupole to iris distance	$\mathbf{m}\mathbf{m}$	340
Cavity active length	$\mathbf{m}\mathbf{m}$	745
Iris to iris distance	$\mathbf{m}\mathbf{m}$	540
Centre to centre between cavities	mm	1285

Table 34: High beta cryomodule and medium beta cryomodule parameters, November 14, 2011.



Figure 91: Schematic partial view elliptical cryomodule slots in the 2011_11_23 linac layout. Top: High beta. Bottom: Medium beta.

4.7 High Energy Beam Transport

The High Energy Beam Transport for the ESS [104] is divided into four sections with their own separate functions. Figure 92 shows a schematic of the HEBT with its main functionalities, consisting of:

- 1. A long (~ 100 m) straight underground section (HEBT-S1) to accommodate space for additional accelerator cryomodules for an energy (that is power) and/or reliability upgrade [105] and, in addition in the beginning of the HEBT, a collimation system.
- 2. A semi-vertical section denoted HEBT-S2 bringing the beam from the underground linac tunnel to the target level at a height 1.6 m above ground level.
- 3. A third horizontal section (HEBT-S3), which includes the expansion system designed to match the beam to the requested footprint on the target.
- 4. A short horizontal section for a beam dump to be used for accelerator tuning and commissioning.

Note at the extreme right in Figure 92 the target monolith and the proton beam window, both with thick shielding. We also observe the neutron catcher absorbing the intense back-streaming neutron beam from the target and the commissioning beam dump used for initial commissioning and daily tuning of the linac. A collimation system is proposed in the beginning of the HEBT, which in addition to the obvious collimation advantages also allows us to reduce the HEBT magnet apertures. Normal conducting magnets are planned throughout the HEBT, and an admittance of roughly $15 \text{rms}_{x,y}$ is obtained with quadrupole apertures of 40 mm radius.



Figure 92: Schematic layout of the HEBT.

The transport system with its magnets has been designed and optimised to obtain the desired beam sizes and Twiss parameters at specified locations. Simulations have been performed using TraceWin with multi-particle simulations of 100,000 particles. Space charge is included in all simulations, although it has almost no effect on the transverse profiles and only minor effects on the longitudinal ones. The layout, horizontal and vertical beam envelopes, and vertical dispersion function for the designed HEBT lattice are shown in Figure 93.

4.7.1 Main sections S1, S2, and S3

Straight section S1 for future cryomodules and collimation. A straight underground section, S1, of around 100 m starting immediately at the exit of the linac is designed as a continuation of the linac focusing structure although non-cryogenic. In this way, installation of future cryostats for power, energy and reliability upgrades is facilitated. Keeping the linac focusing structure in S1 is also expected to minimise the development of beam halo. Still, it is aimed to install a transverse collimation system immediately in the beginning of the HEBT to remove possible beam halos generated in the upstream linac and subsequently reduce losses in the downstream HEBT, see section 4.6.5.



Figure 93: Top: The layout of the HEBT. Middle: RMS beam sizes – horizontal (blue line) and vertical (red line). Bottom: The vertical dispersion function. The beam sizes and dispersion function are based on envelope calculations.

The semi-vertical bending section S2. The section S2 will transport the beam from the 10 metres underground section, S1, to the target level 1.6 metres above ground. Having a system of two double bends $(2 \times 15 \text{ degrees})$ and a FODO-like structure in between. A vertical dispersion of less than 2.3 m is introduced, but the 5 quadrupoles in the uphill part will keep the S2 overall achromatic, as shown in Figure 93 (bottom).

The expander and matching system S3. After the beam has been brought up to the target level, another straight section S3 transports the beam onto the target. In addition to the actual transport, the system is designed to match the required beam footprint on the target, which is assumed to be ± 70 mm horizontally and ± 25 mm vertically. The designed beam envelopes will include 99% of the beam intensity in each direction on the above target footprint. Two separated vacuum systems will be introduced in S3 to separate the target area from the accelerator vacuum system. A proton beam window, provided by the target group, will be needed. Since the proton beam window is positioned upstream of the target, the beam current density at this element will be even higher than at the target, calling for a challenging design.

Quadrupole beam expansion Two beam expansion systems have been designed for the S3 baseline [106], the first being a simple quadrupole beam expansion system, as shown in Figure 93. A simple quadrupole defocusing quartet produces the desired beam profile on the target. Creating a Gaussian profile of the beam in both dimensions results in a relatively high maximum beam current density (around 160 μ A/cm²) with wide

tails and a large power ($\sim 1\% = 50$ kW) outside the nominal target area in either plane. The beam footprint obtained by this method is shown in Figure 94 (left).



Figure 94: The beam foot print obtained at the target from multi-particle simulations of 10^5 particles. Left: By quadrupole expansion. Right: By octupole expansion. The colour scale (representing particle density) in each case is scaled to the maximum value.

Octupole beam expansion. The lifetime of the target is expected to be highly dependent on the beam footprint, that is both the beam peak current density and gradient, but also the extent of beam tails. For the foreseen horizontally slowly rotating target wheel, we see no significant advantage of reducing the tails (as compared to a Gaussian distribution) in the horizontal plane, whereas any reduction of the vertical tails and increase in the flatness of the distribution is expected to augment the target lifetime. Thus, we are proposing a profile, which is Gaussian in the horizontal direction and flat in the vertical direction. Such a profile can be obtained by inclusion of magnetic octupoles. The beam envelopes and intensity distribution at the target obtained with the addition of octupoles are shown in Figure 94 (right panel), showing the obtained flat vertically folded beam profile. A reduction in the maximum beam current density to around 80 μ A/cm² on the target is obtained by this system, and ideally no long reaching tails will exist in the vertical direction. Obtaining this distribution requires two 1 metre long octupoles, an additional quadrupole, and it adds ~ 10 m to the length of S3. Clearly, systems giving flat distributions in both directions can in principle be designed, we do not find the additional complication and risk justifiable.

4.7.2 Collimation

The aim of the ESS accelerator is to provide an intense proton beam on target, but inevitably some of the protons will be lost and a strategy for how and where these losses will occur has to be developed in order to keep the maximum beam loss below 1 W/m for hands-on maintenance. The present discussion will only include very first considerations. The first point is to have a collimation of the beam early in the accelerator system at low energy at the MEBT, in order to provide a beam as clean and without halo to the linac. Next, no collimation is considered in the linac itself, as the aperture in the superconducting cavities is relatively large for other reasons. The associated cold magnets in the linac will have correspondingly large apertures. Hence, the first chance to introduce a collimation system is in the beginning of the HEBT.

In addition to capturing the halo of the beam, the collimators will additionally accept single short stray pulses, and will additionally be used as a diagnostics tool. Two horizontal and two vertical collimation systems are planned, whereas no longitudinal collimation systems are foreseen for the HEBT due to the small beam energy spread ($\Delta p/p \lesssim 0.13\%$) and small dispersion of the beamline. The small dispersion and energy spread make it not only difficult but presumably also unnecessary to include a momentum collimation system.

In order to produce an effective transversal collimation system, a set of two horizontal and two vertical collimators, each consisting of a left/right or upper/lower collimator, positioned with a phase advance of around 90 degrees apart, will be installed in the beginning of S1. Each collimator jaw-system will be designed for 0.5 kW, thus being able to withstand 0.1 ms long single stray pulses. The sacrifice of inserting these collimators is losing lattice cells, which could otherwise be used for future cryostats. Finally, potential beam tails formed in

the HEBT will be caught by a set of fixed collimators just before the proton beam window, which are needed to protect the edges of both the proton beam window and the main target.

4.7.3 HEBT tuning beam dump

A relatively small beam dump for initial commissioning of the linac and for future daily tuning will be installed in the line of sight of S1. The HEBT beam dump line will include a simple quadrupole expansion system analogous to the baseline S3 quadrupolar expansion system. A reduced beam power of 50 kW will be obtained at the dump by a combination of a lower repetition frequency (1 Hz) and a shorter pulse length (maximum 400 μ s at 2.5 GeV). No significant changes in the beam due to RF beam loading et cetera are expected after a few tens of μ s.

4.7.4 Magnet systems

The HEBT will include a large number of magnets with associated power supplies. In addition to the conceptual design of the HEBT, at present a study is ongoing on the technology to be used in these magnet systems, considering the use of normal conducting magnets as well as low- and high-temperature superconducting magnets. The study will also include lifecycle aspects by minimising total costs including operational costs over a 10 year period. The baseline HEBT design in HS_2011_11_23 contains the list of the main magnets shown in Table 35. A number of power converters will supply the DC currents used by the magnets. These units are designed for high efficiency, but reliability aspects will also be considered at the outset. Several minor elements as steerers and their associated power supplies will clearly also be needed.

Special issues apply for the magnets in the S3 section, as these magnets are exposed to a high radiation dose. Consequently, special materials will be employed in addition to provision of remote exchange of these magnets.

Parameter	Unit	Value
Dipole count		4
Dipole length	\mathbf{m}	2.8
Dipole aperture, horizontal	$\mathbf{m}\mathbf{m}$	80
Dipole aperture, vertical	$\mathbf{m}\mathbf{m}$	40
Quadrupole count		25
Quadrupole length	m	0.4 or 0.6
Quadrupole aperture, radial	$\mathbf{m}\mathbf{m}$	40
Octupole count		2
Octupole length	m	1.0
Octupole aperture, radial	$\mathbf{m}\mathbf{m}$	40

Table 35: Main magnets for HEBT.

4.8 RF Systems

The RF system converts AC line power to RF power, to be supplied to the RF accelerating cavity couplers. The AC conventional power lines on one side, and the waveguide power couplers on the accelerating cavities on the other side, bind the scope of the RF system.

The linac reaches an energy of 2.5 GeV within 350 metres, corresponding to an average gradient of 7.1 MV/m, delivering an average power of 5 MW with a 4% duty factor (2.9 ms pulse at a 14 Hz repetition rate). Thus the peak power is over 123 MW. This averages to a peak power density of over 350 kW/m, an unprecedented value. Because of the large power density, 98% of the linac consists of superconducting RF resonators that transfer power to the beam. The normal conducting linac is powered by four power sources, one for the RFQ and the bunching cavities in the medium energy beam transport and three power sources for the three drift tube tanks. There are three types of superconducting resonators – spoke resonators that operate at 352.21 MHz and elliptical cavities operating at 704.42 MHz. Table 36 shows the list of power sources that drive these cavities. As shown in Figure 95, the power level covers a range from 50 kW to 950 kW.

Module	Frequency [MHz]	Quantity	Max. power to coupler [kW]	
RFQ	352.21	1	1000	
DTL type A	352.21	1	2100	
DTL type B	352.21	2	2100	
Spoke	352.21	36	250	
Elliptical medium- β	704.42	64	610	
Elliptical high- β	704.42	120	950	



Table 36: List of required RF power sources.

Figure 95: Power supplied to the beam versus superconducting resonator index number.

4.8.1 RF system design

The RF system determines the specifications for the RF subsystems such as the low-level RF, RF distribution, et cetera. Tables 37 and 38 show requirements and specifications for the RF system.

Requirements. Three factors indicate that tolerances on RF control are not as stringent as at other high power facilities:

- 1. The linac uses protons instead of H^- ions.
- 2. The linac does not inject into a ring
- 3. The linac is heavily coupled due to its high beam current, and has a large system bandwidth.

Parameter	Unit	RFQ	Buncher	DTL	Spoke	Med.	High
						β	β
Number of couplers		1	2	3	36	64	120
Average coupler spacing	[m]	0	1	7	2.1	1.8	1.8
Max. power delivered to coupler	[kW]	1000	10	2100	245	610	950
Min. power delivered to coupler	[kW]	1000	10	2100	100	50	610
Ave. power delivered to coupler	[kW]	1000	10	2100	215	400	900
Max. reflected energy per pulse	[J]	150	2	315	500	1100	1700
Frequency	[MHz]	352	352	352	352	704	704
Average synchronous phase	[degrees]	0	90	30	15.2	15.9	14
Loaded Q	$[10^3]$	15	15	15	160	640	820
Maximum cavity fill time	[uS]	50	50	50	400	250	250
Lorentz de-tuning coefficient	$[Hz/(MV/m)^2]$	0	0	0	1	1	1
Lorentz de-tuning time constant	[ms]	0	0	0	1	1	1
Slow tuner range	[kHz]	100	100	100	100	100	100
Slow tuner slew rate	[kHz/s]	1	1	1	1	1	1
Maximum slow tuner cycles	$[10^{6}]$	1	1	1	0.1	0.1	0.1
Fast tuner range	[kHz]	0	0	0	10	10	10
Fast tuner bandwidth	[Hz]	1	1	1	1000	1000	1000
Cav. phase noise (microphonics)	[Hz]	0	0	0	10	10	10
Cavity drift rate	[Hz/s]	1	1	1	1	1	1

Table 37: RF system requirements.

Parameter		RFQ	Buncher	DTL	Spoke	Med.	High
						β	β
RF regulation overhead	[%]	25	25	25	25	25	25
RF distribution loss budget	[%]	5	5	5	5	5	5
RF pulse Length	[ms]	2.91	2.91	2.91	3.26	3.11	3.11
Number of couplers per power source		1	1	1	1	1	1
Saturated RF power per power source	[kW]	1300	15	2750	350	800	1250
Minimum efficiency at operating power	[%]	43	43	43	50	47	47
Number of power sources per modulator		1	3	1	9	3	2
Max. modulator stored energy per pulse	[kJ]	6.8	0.2	14.5	14.5	12.5	13
Modulator efficiency	[%]	95	95	95	97	95	95
Total average AC power	[kW]	100	2	650	750	2500	10550
Total average cooling rate	[kW]	59	1	400	400	1400	5850

Table 38: RF system specifications.

The RF systems provide RF power for 50 mA of peak beam current for a pulse length of 2.86 ms at a pulse rate of 14 Hz. The fill and fall times of the cavities are on the order of 300 μ s, so the total RF pulse length is approximately 3.5 ms and the total duty factor is 4.9%. The regulation of the voltage amplitude is less than 0.1% with a phase error of 0.5 degrees. The design accommodates variations on the order of 5% in cavity-to-cavity coupling strength and Lorentz detuning factors.

Design. A schematic of a klystron RF station is shown in Figure 96. The baseline configuration has one cavity per power source, meeting the tight requirements on cavity gradient and accommodating the variations in cavity-to-cavity coupling strength and Lorentz detuning factors. A conservative value of 5% is assumed for the insertion loss – the power loss from the power source to the resonator. Similarly, a value of 1.25 is taken for the power overhead factor – the ratio of the maximum output power of the RF source to the operating power. This overhead factor is necessary for the regulation to work properly. Taken together, insertion loss and power overhead indicate that the RF power source needs to make available 1.3 times more power than the required beam power. Thus the range in power sources is from 65 kW to 1100 kW for the superconducting cavities, and 1200 kW to 2600 kW for the normal conducting cavities.





Figure 96: System block diagram of a klystron RF system, with one cavity per power source.

Figure 97: Forward and reflected power at the cavity coupler for coupler design set at optimum coupling for 50 mA of beam current and maximum cavity voltage.

The bandwidth of the system is dictated by the loaded cavity bandwidth. The power coupler is designed to transfer all RF energy to the beam passing though the cavity, with an optimum coupling value at a unique

Module	Source output power [kW]	R/Q [Ω]	$egin{array}{c} Q_{external} \ [{f 10}^3] \end{array}$	Bandwidth [kHz]
RFQ	1300			
DTL type A	2800			
DTL type B	2800			
Spoke	350	500	160	2.2
Elliptical medium- β	800	300	640	1.1
Elliptical high- β	1250	477	820	0.9

Table 39: Overview of RF power sources.

cavity voltage, beam current and R/Q. The baseline design uses 50 mA for the beam current and the maximum voltage for each type of cavity. Figure 97 shows the forward and reflected RF power for the different cavity voltages. The loaded Q's and bandwidths are shown in Table 39.

4.8.2 Low Level RF control

The LLRF control system controls and maintains the amplitude and phase stability of the accelerating fields in pulse mode for all the RF cavities along the linac (RFQ, DTL, Spoke cavities, medium beta and high beta cavities), with one power source driving one cavity. General requirements of the LLRF system are shown in Table 40.

Requirements. The power overhead for LLRF control is specified by the RF system design. The degree of automated operation is also specified. There is one power source driving each individual cavity.

Design. The LLRF system uses a combination of feedback and feed-forward. The feedback system is centred on a PID-controller. Adaptive feed-forward control is used to compensate for the droop and ripple of the klystron modulators. Feed-forward linearisation, or pre-distortion, will be investigated in order to minimise the headroom necessary in the klystrons. The LLRF system also controls the slow tuners and the fast piezo-electric tuners that are fitted to the superconducting cavities. Adaptive feed-forward control also compensates for the effects due to Lorentz detuning.

The LLRF system uses an analog down- and up-mixer, with all the processing and automatic control performed at baseband. This is possible in the digital domain, preferably on an FPGA platform with the benefit of being reconfigurable by software, and thus adaptable for current and future needs. The same baseband electronics works for the whole linac, with only the up and down converter boards being adapted to either 352 MHz or 704 MHz operation.

The LLRF design phase will generate a list of specifications that will be needed for procurement, and to influence other systems. For example, the LLRF will require power overhead for regulation, and will also specify the maximum phase noise, phase drift from clock and reference system, maximum ripple in modulator, the maximum detuning of the cavity, the interface with control system, et cetera.

Parameter	Unit	Value
Maximum beam current	[mA]	50
Beam current stability	[%]	1
Beam current control	[%]	1
Beam current ripple	[%]	1
Beam current pulse length	[ms]	2.86
Beam current pulse length stability	[ppm]	1
Beam current pulse length control	[ppm]	1
Repetition rate	[Hz]	14
Cavity gradient amplitude regulation	[%]	0.5
Cavity gradient phase regulation	[deg.]	0.5
Allowed AC grid load variation (flicker)	[%]	1

Table 40: General requirements of the LLRF system.

4.8.3 Master oscillator

The master oscillator is responsible for generating both the reference phase for the RF systems, and also the master clock for the control system. These two time references are phase locked to each other.

Requirements. The requirements for the master clock come from the controls. The requirements give the phase noise and long-term stability of the system.

Design. The master oscillator is slowly locked to the GPS system, and is used to generate the necessary RF reference frequencies and control system clocks and timestamps. The need for redundancy is being investigated. The master oscillator subsystem is interfaced to the control systems by the EPICS interface.

The phase reference is a common master oscillator for the whole linac, which synthesises the LO necessary for the 352 MHz and 704 MHz parts. The master oscillator provides the control system with a UTC clock that is phase locked to the phase reference for the linac. An oven controlled crystal oscillator gives the necessary low phase noise for the linac operation. It is phase locked to a caesium clock in order to control the slow drift. The caesium clock is locked to the GPS system. The control system clock is derived from the crystal oscillator, and not from the caesium clock, in order to have the local time stamps phase locked to linac operation. Thus it will differ from the actual UTC time only by only a finite amount, at any given moment. The absolute size of the difference is kept below 0.1 sec.

4.8.4 Phase reference distribution

The phase reference distribution takes the RF signal(s) from the master oscillator and distributes them to the separate RF systems. The system starts at the output of the master oscillator and ends at the inputs of the LLRF systems.

Requirements. Phase stability requirements come from the RF systems design. The exact requirements of the phase distribution are derived from this and from the performance of the master oscillator.

Design. The central concept is a phase stable coaxial line in the linac tunnel, with taps at each LLRF feedback point going up to the klystron gallery. This reference line is temperature controlled and gas filled, in order to minimise drift. A possible alternative is to use a fibre optic phase distribution scheme. The specifications include the cabling, the connectors and/or taps, the heat stabilisation systems, et cetera. The connections to the subsystems are also specified, both electrically and mechanically.

4.8.5 **RF** power sources

The RF power source system is the collection of amplifiers that takes signals from the LLRF system and generates high power RF signals, then supplies them to the RF distribution system. These amplifiers are typically klystrons, although tetrodes or induction output tubes (IOTs) can be used for the low frequency and lower power sub-systems. The RF power source system also includes driver amplifiers that generate RF power at a level appropriate for the final amplifier.

Requirements. The number of power sources and their power levels are specified from the beam physics design, while the RF power overhead is specified from the RF system design. One power source per cavity provides the required regulation over the long beam pulse. The sources accommodate a 3.5 ms long pulse length with a duty factor of 4.9% The design considers the RF frequency and power level required for each type of RF load. The maximum power saturated power required is shown Figure 97.

Design. The design determines which type of power source is used – klystron or IOT, for example. Frequency and power requirements limit the choice to power vacuum tubes, because solid state amplifiers do not have the peak power reach for the linac design, at this time. Each power source is an amplifier and not a locked oscillator, in order to meet the amplitude and phase stability requirements.

Gridded tubes. Gridded tubes – tetrodes or IOTs – are an attractive choice at low power and at low frequency (352 MHz), because of their high efficiency (60% - 70%). They have rather low gain (~ 20 dB), so that high power solid state drivers or tube amplifiers are needed to drive the final output power tube. The maximum frequency of a gridded power tube is less than 500 MHz, because of transit time limitations.

Klystrons. Klystrons are high power electron tubes that use a drift tube to convert a modulation of electron velocity to a modulation of electron density. This permits them to operate at very high frequencies and very large peak powers; well into the tens of GHz and tens of MW ranges. However, they do so with

less efficiency than a gridded tube (50 - 60%), and the drift tube and coupling cavities become prohibitively large at lower frequencies. The gain of multiple cavity klystron is very large (> 40 dB), eliminating the need for expensive driver amplifiers. The baseline design uses only pulsed klystrons, without an anode modulation terminal, because they are less expensive and more reliable.

Drift tube linac and spoke cavities. High power levels on the order of 1 MW-2 MW are required for the 352 MHz drift tube linac, limiting the power source choice to a klystron. There are multiple vendors who can produce these klystrons. In contrast it would be uneconomical to use a klystron for each 352 MHz spoke cavity. A number of tetrodes on the market have the required power for the spoke cavities. Although not many IOTs have the peak power range for the spoke cavities, it is possible to combine two IOTs. A driver system is also needed with a gridded tube solution.

Elliptical cavities. The maximum saturated power required at 704 MHz ranges from 200 kW-1100 kW. The baseline design uses a single klystron design with a maximum saturated output power of 1.1 MW, because of the large number of power sources and because of the desire to simplify procurement and operation. There is only a small number of vendors, and the vendor lead-time is long.

4.8.6 Modulators

Klystrons and gridded tubes are energised by modulators that convert conventional AC power into pulsed power. These modulators operate at fairly high voltages, because most of the RF power sources are electron tubes.

Requirements. RF power source specifications form the main body of requirements for the modulator – voltage, current, voltage droop, ripple, et cetera. Beam physics constraints such as pulse length and cavity fill time also place additional requirements. There is also a requirement on the amount of variation the modulator load can put back on the power grid (flicker).

The modulators are small enough to fit into the klystron gallery. At the high energy end of the linac the modulators are able to power at least two 1.1 MW klystrons per modulator, with one klystron per elliptical cavity. This same modulator design is also able to power a single 2.8 MW klystron. This ability leads to a cost saving, since the cost of providing energy storage is about 50% of the cost of a modulator – a modulator powering two klystrons will be about 25% cheaper than two modulators each powering a single klystron. However, there is a limit to how much energy a modulator can store. The baseline design limits the stored energy to 20 kJ per pulse.

Design. The design uses solid state pulsed modulators with integrated arc protection capability, and excludes HV tube crowbars. There are a number of different solid state pulsed klystron modulators suited for long pulse applications. Some of the topologies they use are shown in Figure 98. Each type of modulator is available from industry and will meet the baseline specifications.

The modulator voltage is typically 110 kV, with a current of about 17 A, for a 1.1 MW klystron operating at an efficiency of 60%. This corresponds to a stored energy of about 6.5 kJ per pulse. In comparison, a 2.8 MW klystron operating at 58% efficiency uses a modulator voltage of typically 110 kV, and a current of about 44 A, with a stored energy of 17 kJ per pulse. Thus, a single modulator design for a single 2.8 MW klystron in the 352 MHz drift tube linac can also power at least two 1.1 MW, 704 MHz klystrons in the high energy end of the linac.

The design requires more than 110 modulators, so the modulator construction rate exceeds two modulators per month in order to meet a 4.5 year construction schedule. A production rate of one modulator per production line per year indicates the need for 24 lines operating simultaneously. This is beyond the current capacity of modulator manufacturers. This problem can be tackled by a number of different strategies:

- 1. Use multiple manufacturers, each using their own topology.
- 2. License a single topology from a given manufacturer, and subcontract the design to other vendors.
- 3. Develop an open source design and have multiple vendors build-to-print.

The "multiple topology" strategy (1) is unattractive because of the many different types of modulators to operate and repair during operations, with a large pool of spare parts. The "single license" solution (2) makes operations and repair more manageable, and enables the primary vendor to manage the entire procurement. However, problems with technology transfer between vendors could lead to single point of failure. The "open source" solution (3) avoids single point failures, but will require an extra management burden on ESS during procurement, and requires a prototype to be built to prove the open source design. The current plan is to use this solution; to develop an open source design and to have multiple vendors build-to-print.



Figure 98: Various modulator topologies. The monolithic pulse transformer topology is a proven technology. Another attractive option is the resonant modulator topology.

The monolithic pulse transformer topology shown in Figure 98 is a proven technology that has been successfully employed at a number of long pulse linacs. This would be a good choice for an open source design. However, the long pulse makes the pulse transformer rather bulky. Another attractive option is the resonant modulator topology. This topology is more modular and avoids a large pulse transformer, which could be a single failure point. The current strategy is use the monolithic pulse transformer modulator for the first set of modulators. A prototype of this design can be built rather quickly, because of its long history. The resonant modulator is also being pursued in parallel, but the prototyping will take longer. The resonant modulator will be used for the second series of modulator procurements.

4.8.7 RF distribution

The power distribution system transports RF energy from the power sources through the tunnel penetrations to the various accelerating resonators. The distribution system encompasses all components from the outputs of the power sources to the inputs of the cavity couplers.

Requirements. The requirements include the amount of power that the system is capable of handling, including the overhead specified by the RF system design and the output power of the power sources. The insertion loss of the system does not exceed 5%. Arc detection and other safety and machine protection issues are being addressed. The system includes directional couplers for use in low level RF control and power source protection.

Design. The distribution system consists of stretches of WR1150 waveguide from the output of the power source through the tunnel penetration, including appropriate waveguide bends, et cetera, to direct this power by the most reasonable route. Significant emphasis is placed on keeping the total waveguide length to a minimum, although emphasis is also placed on maintaining the simplicity of the overall system. The design therefore involves a repetitive structure, and minimises the number of unique layouts.

The reactive impedance that a cavity presents to the power source when the cavity is being filled or emptied reflects RF energy. Similarly, RF power is reflected back from the cavity coupler during the beam pulse, if the cavity coupling is not fully optimised. A circulator that deposits the reflected energy in a load protects the power source from reflected power during normal operations and system faults.

The distribution system includes a number of directional couplers for use in low level RF control and in power source protection. The WR1150 waveguide is protected against arc faults by filling it with slightly over pressurised dry air. Higher peak fields are expected within the circulators, which are therefore filled with SF6 as an insulating medium. Such "off the shelf" components are found in many manufacturers catalogues as entirely enclosed devices. Arc fault detection systems and other machine protection devices are connected to the interlocks provided by the LLRF system, to prevent significant system damage. The baseline design, with one power source per resonator, removes the need for additional RF vector control beyond that already supplied by low level control of the power sources.

4.8.8 RF equipment gallery

The RF equipment gallery contains a integrated array of systems, ranging from low level RF control to high power RF sources such as klystrons. The power sources and the modulators are supported by a large amount of infrastructure, such as cooling water and AC power. The RF distribution system comprises a complex system of waveguide components.



Figure 99: Possible layout of a section of the equipment gallery, with one klystron per modulator.



Figure 100: Equipment gallery layout with two klystrons per modulator.

Requirements. The requirements for the gallery are driven by specifications from the power source, modulator, distribution and low level RF systems.

Design. The design takes into account the conventional facility requirements and the physical space requirements. The physical footprint of the modulator is quite large, because of the high voltage and the large amount of stored energy. This large footprint makes it difficult to have enough space in the high beta section of the gallery for a single modulator per klystron, in the configuration shown in Figure 99. Substantial space is made available if a single modulator powers two klystrons, as illustrated in Figure 100.

Klystrons operate at efficiencies of 50%-60%, depositing a large amount of power into the klystron collectors, and into the cooling water system. The cooling water temperature increases by (typically) 7 C as it passes through a klystron collector when the klystron is operating at maximum saturated power, and by about 14 C if no RF power is generated. It is possible to cool four klystrons in series with an inlet water temperature at 40 C, always ensuring that the maximum collector temperature does not exceed 85 C. The water temperature is about 70 C after the fourth klystron, in the useful range for recycling recovered heat into the district heating system.

4.9 Cryogenics

ESS will use cryogenics in at least three different parts of the machine, namely the linac, the target and the experiments including instruments. Additionally, cryogenics might be used in test stands, workshops and laboratories. Each of these systems presents its own special challenges linked to the nature of the client. The common challenges faced by all systems include energy efficiency, investment costs, running costs, and availability/reliability/operational stability.

The cryogenic system concept is based on separate cryoplants to cater for the liquid helium (LHe) needs as well as a delivery based solution for liquid nitrogen (LN2). There are four separate subsystems:

- 1. Linac cryogenic system:
 - (a) A 2 K helium cryoplant, supplying liquid helium to the accelerators superconducting RF (SCRF) cavities which are located in the cryomodules;
 - (b) An associated transfer line, distributing the helium at 4.5 K to the cryomodules valve boxes;
 - (c) Valve boxes situated on or near each cryomodule, controlling the flow of helium into and out of the respective cryomodule, converting the 4.5 K helium to 2 K helium;
- 2. Target cryogenic system:
 - (a) A helium cryoplant, supplying helium at around 18 K to the hydrogen system of the target moderators;
 - (b) An associated transfer line, transporting the helium to the hydrogen system;
 - (c) A 20 K hydrogen system, using the 18 K helium to cool hydrogen and circulating the hydrogen in the target moderators;
 - (d) Associated transfer lines, distributing the hydrogen to the target moderators;
 - (e) Note that the target moderators themselves are not part of the supply!
- 3. Central liquefier system:
 - (a) A helium liquefier, supplying liquid helium by batch to the instruments comprising an integrated purifying system and high pressure storage;
 - (b) A system of fixed and mobile dewars, storing and distributing the liquid helium to the instruments as well as to cryogenic test stands and other small clients;
 - (c) A warm helium return pipe, collecting warm used helium from the instruments, transporting it to the liquefiers integrated purifying system;
- 4. Liquid nitrogen system:
 - (a) A system of fixed and mobile dewars, receiving the liquid nitrogen from commercial suppliers trucks, storing and distributing it to the instruments as well as to cryogenic test stands and other small clients.

This chapter describes the refrigerators for the linac and the target including their distribution transfer lines as well as the liquefier for the instruments. The liquid nitrogen supply system are not described in any detail.

4.9.1 Linac

The clients of the cryogenic system in the linac are the superconducting RF (SCRF) cavities which are located in the cryomodules. A preliminary extrapolated heat load estimate for the linac, including distribution, shows a total equivalent heat load of around 14 kW at 4.5 K. For more reliable numbers, a bottom-up heat load inventory is needed.

4.9.2 Cryoplant

Cooling in a steady-state process is done by allowing a working fluid to undergo a series of cyclic thermodynamic transformations, of the multitude of possible useful thermodynamic cycles, the prevailing process arrangement for a large 4.5 K helium refrigeration plant is the Claude cycle, a combination of the Brayton and Joule-Thomson cycles. For very high cooling capacities it is advantageous to design a sophisticated Claude cycle with multiple expanders and a complex flow distribution in the heat exchangers. The ESS linac cryoplant will be similar to an LHC cryoplant, as shown in Figure 101, with roughly the same layout, but somewhat smaller in size and power.



Figure 101: Cold box of Linde 4.5 K LHC refrigerator.



Figure 102: Coefficient Of Performance of large cryogenic helium refrigerators.

Designing an energy efficient refrigerator is achieved not only by improving single components, but by the arrangement of these components in a carefully optimised cycle. The equivalent capacity, expressing the total cooling capacity as equivalent isothermal refrigeration at 4.5 K, is used to compare capacities of cryogenic machines. The ratio of overall power consumption versus the cooling produced, Coefficient Of Performance (COP), of the 4.5 K refrigerators at CERN is about 220 or 30% of the Carnot cycle. Figure 102 illustrates the variations and spread of COP for different types of large scale cryoplants. The LHC/LEP and HERA plants deserve a closer look during the conceptual design of the cryoplants, because of their similarity in client load demands and their exceptional efficiencies.

Refrigeration cycles. Most modern helium refrigeration cycles do not use liquid nitrogen pre-cooling on a permanent basis. A 2 K refrigerator uses a 4.5 K refrigerator as a starting point. The 4.5 K liquid helium is cooled to just above its superfluid transition at 2.17 K, before expansion down to 2 K. Large capacity refrigeration at 2 K requires the use of cold compressors on the low pressure return line. There are two possible principal layouts, as illustrated on the left of Figure 103: (i) the integral cycle with cold compressors pumping the helium all the way from the millibar range up to atmospheric pressure and (ii) the mixed compression cycle with its volumetric warm compressor. The mixed compression cycle appears to be better suited for large dynamic ranges and for good downturn efficiency.



Figure 103: Refrigerator cycles. Left: Two possible principal layouts in a CERN study on 2K cycles. Right: A TESLA model refrigerator delivering 4.25 kW at 2K.

The LHC 1.8 K refrigerators achieve a COP slightly less than 1000 at 100% refrigeration capacity, and about 1600 at 40% capacity downturn. The COP of the TESLA-style refrigerator cycle shown on the right of Figure 103 is around 720 or 21% of Carnot at 1.8 K, at maximum capacity.

Compressors. Cold compressor and screw compressor optimum pressure ratios and dynamic range are key factors in designing highly efficient 1.8 K mixed cycle cryoplants. The maximum size of a 2 K refrigerator is driven mostly by the maximum flow achievable by the cold compressors. A typical helium cryoplant in the multi-kilowatt range has the following layout:

- 1. Compressor station
 - (a) oil-injected screw compressors, multi stage
 - (b) capacity control by slide valve

- (c) oil removal: three stages of coalescing filters and charcoal bed absorber
- 2. Coldbox
 - (a) brazed aluminium plate-fin heat exchangers
 - (b) cold turbo expanders with helium bearings
- 3. Cold turbo compressors
- 4. Gas storage for complete helium inventory (warm)

Cryogenic distribution. The proposed cryomodule design requires that the cryogenic distribution is located outside the cryomodules in a separate transfer line (TL). The linac TL will be around 450 m long, of which 390 m are the length of the cold linac and 60m the length of the TL from the coldbox to the linac tunnel. There will be valve boxes and jumper connections to supply each of the 45 cryomodules. With a client requiring helium at 2K, there are two options for its distribution:

- 1. Liquid helium flows through the TL at 4.5 K this requires separate heat exchangers and expansion valves for each of the cryomodules, limiting heat load by using a higher temperature;
- 2. Liquid helium flows through the TL as saturated superfluid helium at 2 K, requiring only one central expansion valve, increasing heat load by using 2 K along the whole TL; The baseline is distribution at 4.5 K, but further studies are necessary to corroborate this choice.

Experience shows that a typical specific heat load for a robust TL is not higher than 1 W/m at 4.5 K. The heat load of the jumper connections and valve boxes is not known and depends highly on specific design choices, but can be estimated to be less than 150 W in total (based on the assumption that a singularity in the TL contributes the equivalent of ca. 3 m of normal TL). The total heat load of the linac distribution is therefore estimated at 600 W at 4.5 K. These numbers need to be verified in further studies, and can only be confirmed when the detailed design and engineering of the distribution system are finished.

4.9.3 Target

The cold moderator cooling circuit (CMCC) is a cryogenic helium circuit which is the cold source for the two cold moderator hydrogen circuits (CMH2) [107]. Requirements related to cold moderator hydrogen circuits are to keep the hydrogen temperature of 20 K (at 5 MW) and the pressure of 1.5 MPa constant during ESS operation, including ramping up of the proton beam power from 0 to 5 MW.



Figure 104: The SNS target moderator cryogenic system.

The layout of the target moderator cryogenic system shown in Figure 104 follows the concept of the SNS moderator system wherever possible. The SNS system cools 3 parallel hydrogen moderator vessels with a supply temperature of 20 K and a continuous combined heat load of 7.5 kW, with an operating pressure of 14 to 15 bar (1.4 to 1.5 MPa) when the beam is off and 15 to 16 bar when the beam is on. The helium coldbox design is fairly simple, compared to cryoplants for lower temperatures, containing one regenerative heat exchanger, a 20 K absorber one turbine and a turbine cooler. The helium-hydrogen heat exchangers are plate-fin type. The hydrogen is circulated by fan type impellers mounted in diffusers. The system has passive bellows (accumulators) that expand and contract as the system volumes change when the beam is turned on or off.

4.9.4 Instruments

The estimation of liquid helium (LHe) and liquid nitrogen (LN2) needs for the instruments, listed in Table 41, is interpolated from the consumption at ILL. The full set of instruments will use 17 l/h of LHe in normal operation with a peak load of 35 l/h or an average load of around 100,000 l/year. The LN2 consumption will be around 200 l/h or 1500 m³/y.

Parameter	Unit	Value
Annual consumption of liquid nitrogen	$\mathrm{m}^3/\mathrm{year}$	1,500
Annual consumption of liquid helium	l/year	100,000
Instrument liquid helium usage rate, normal operation	l/h	17
Instrument liquid helium usage rate, peak	l/h	35
Liquefaction rate at rise level, without LN2 pre-cooling	l/h	45
Optional peak liquefaction rate, with LN2 pre-cooling	l/h	90
Liquid helium storage capacity	1	5,000
Maximum liquefier operation time, per year	h	7,500

Table 41: Cryogenic plant parameters for instruments.

Liquid Helium Supply. This LHe consumption of several tens of thousands of litres per year necessitates an onsite liquefier and recovery system. The price of helium gas being nearly the same as for LHe (per mass) only the operation of a liquefier in combination with an efficient recovery system is reasonable. Usually the necessary supply of 5 to 10 % helium losses during one circulation is the biggest running cost, hence a well organised recovery is absolutely crucial for optimal use of the liquefier.

Today, state of the art He liquefiers offer a COP of about 12% of the Carnot limit, which translates into 2.3 kWh per litre of LHe. Two overcapacity factors are taken into account when estimating the required rate of LHe liquefaction:

- 1. A factor of 1.5, enabling about 1500 l of "level rise" to be made for every 1000 l to be delivered.
- 2. A factor of 1.7 to cover peak demands and to bridge downtimes due to machine failure or corrective maintenance.

The combined total overage factor of 2.5 indicates that a liquefier capacity of 45 l/h is needed to meet the instrument requirement of 17 l/h. Another key parameter is the liquid storage capacity. A well designed plant should have a large liquid helium storage capacity in order to prevent LHe shortages during downtime. Generally, storage of one week of high liquefaction rate production allows for the necessary flexibility, for a good equalisation capability of peak demands and for a decent capacity to sit out helium supply shortages. Good practice calls for the plant running continuously, rather than operating with regular starts and stops. Continuous operation reduces thermal cycling of the cold box and decreases the risk of malfunctions and is beneficial in terms of energy efficiency. For example, starting from a warm machine, a cool down time of 6 to 8 hours at full power is needed before reaching liquefaction. The annual maximum liquefier operation should be 7500 h.

For a 45 l/h rate, a 5000 litre liquid storage capacity is advisable, enough to also meet occasional peak demands. Most helium liquefiers offer the option to double LHe output by additional liquid nitrogen (LN2) pre-cooling. Typically a flow rate factor of 0.7 (litre LN2 / litre LHe) applies. The benefit lies in the significant reduction of cool-down times (typically 2 to 3 hours less). Such an option can also boost capacity up to 90 l/h to match very high peak loads. A dedicated high pressure LN2 storage tank is necessary.

4.10 Vacuum

This section describes the vacuum requirements for the linac, the target and the instruments, as well as listing some basic considerations concerning the vacuum systems. One of the biggest challenges for the ESS-wide vacuum system is the organisation of the maintenance and the amount of spare parts that need to be stocked. The number of pumps and sensors makes it very important to standardise the equipment wherever possible.

Linac. The vacuum system of the accelerator consists mainly of pumping stations and instrumentation for the beam vacuum. There will be vacuum packages associated with each of the intermodule utility spaces in the cold linac, with certain pieces of equipment in the warm linac, and with lengths of beam pipe in the HEBT. The total number of vacuum packages is estimated to be between 60 and 70. Insulation vacuum for cryogenics is not considered in this section.

Target. The target system requires mostly temporary vacuum for flushing and leak testing. A few systems need permanent vacuum packages.

Instruments. The instruments will all use vacuum, and so will the neutron guides. A summary of the requirements is given in the instruments vacuum list, Table 42.

Parameter	Unit	Value
Number of roughing pumps		165
Roughing vacuum pressure	mbar	$7 imes 10^{-2}$
Number of vacuum pumps		22
Good vacuum pressure	mbar	7×10^{-4}
Total number of pumps		187
Estimated guide volume	m^3	86
Estimated instrument volume	m^3	181
Total volume	m^3	267

Table 42: Vacuum parameters for the instruments.

4.11 Beam Instrumentation

Successful commissioning and operation of an accelerator relies on the availability of proper beam diagnostics. The final beam diagnostics specifications will be fixed in the Technical Design Report. In the meantime, the beam diagnostics requirements for the ESS are preliminarily based on the following assumptions:

- 1. The beam loss monitoring system is sufficiently sensitive to keep average losses at a level where hands-on maintenance is possible, and have enough time resolution/dynamic range to protect the machine from damage by shutting down the source in case of uncontrolled fast beam loss.
- 2. The beam current should be measured at the percent level, or better.
- 3. The beam position needs to be measured with an accuracy of a couple per cent of the beam size. The measurement should have a sufficient time response to be able to observe transients for example in the beginning of the pulse.
- 4. The time of arrival (phase) should be measured to a fraction of a degree of RF phase. A fast response to changes is not needed to phase the cavities, but may be useful for example for LLRF studies.
- 5. The beam size needs to be measured with an accuracy of 10% or better. The measurement can be an average over the linac pulse, although time resolution of the same order as the BPM system would be useful.
- 6. The bunch length needs to be measured with an accuracy of 10% or better. The measurement can be taken as an average over the pulse, or on a single bunch in the train, but there is no need to measure the bunch length of all bunches individually.
- 7. The transverse halo needs to be measured with a sensitivity corresponding to a fraction of the amount of beam that can be lost continuously during operation without excessive activation of the machine.
- 8. The beam distribution on target needs to be measured with an accuracy of 10% of the nominal peak density.

The resulting specifications are summarised in Table 43, along with the values of some other parameters, such as vacuum pressure and beam pipe apertures, which are relevant for the design of beam diagnostics. Clearly, these specifications will evolve during the design update phase. Table 44 outlines the distribution of diagnostics systems in the different parts of the linac, based on an assessment of beam diagnostics needs for the HS_2011_11_23 layout.

Cold versus warm. In the cold linac, warm space is needed for some types of diagnostics, in particular for the longitudinal and transverse profile devices. While developing such diagnostics devices for cryogenic operation is possible, it would require significant additional R&D as well as introduce additional risk. This consideration, along with the desire to minimise the cryogenic load, lead to the hybrid cryomodule concept.

4.11.1 Beam loss

The beam loss monitoring system is arguably the most important diagnostics system, as it provides a critical input to the machine protection system. Therefore it is very important that the system does not have any blind spots. Simulations, which have started and are ongoing, will determine the exact location, number and types of monitors used. The beam loss monitor system will likely use a combination of ionisation chambers, fast PMT-based detectors, and neutron detectors. Scaling from SNS values indicate that a response time of a few μ s is needed, and it seems achievable by modifying the SNS ionisation chamber design. Some beam loss monitors may need to operate at cryogenic temperatures, due to the shielding effect of the cryomodules, and the push to avoid unnecessary warm space. Cryogenic beam loss monitors are being developed at for example CERN and Saclay. Diamond detectors may be an interesting option in those applications.

4.11.2 Beam current

The beam current sensitivity requirement may be achieved using off-the shelf beam current transformers. However, absolute calibration at this level is challenging. Several transformers will be placed in the low energy part, to measure beam transmission. In the high energy end, a beam current transformer will placed at each transition between main linac sections.

Parameter	Unit	Value
BEAM LOSS MONITORS		
Number of BLMs		169
BLM response time	$\mu { m s}$	3
Beam loss sensitivity	W/m	0.01
BEAM POSITION MONITORS		
Number of BPMs		107
Beam position resolution	$\mu { m m}$	100
Bunch arrival time resolution	\mathbf{ps}	4
BEAM CURRENT MONITORS		
Number of BCMs		10
Beam Current resolution	$\mathbf{m}\mathbf{A}$	0.5
SLITS and FARADAY CUPS		
Number of slits		8
Number of Faraday Cups		2
Faraday Cup sensitivity	μA	0.5
TRANSVERSE PROFILES		
Number of Transverse profile Devices	23	
Beam size resolution	%	10
TRANSVERSE HALOS		
Number of Halo Monitors		tbd
LONGITUDINAL PROFILES		
Number of Longitudinal profile devices		12
Bunch length resolution	%	10
BEAM-ON-TARGET MONITORS		
Number of target beam spot monitors		1

Table 43: Beam instrumentation parameters, November 29, 2011.

Section	Beam Loss	Beam Position	Beam Current	Transverse Profile	Emittance	${f Bunch}\ length$	Faraday	Halo
LEBT			2	3	1		1	
RFQ		-	-	-	-	-	-	-
MEBT		4	2	3	1		1	2
DTL	30	3	2					
Spoke	45	30	1	4		3		tbd
Medium β	30	20	1	4		3		tbd
High β	42	28	1	4		3		tbd
HEBT	22	22	1	5		3		tbd

Table 44: Overview of current instrumentation plans in the HS_2011_11_23 layout.

4.11.3 Beam position and phase

The beam position system will likely use buttons, except in the front-end where shorted striplines may be used, particularly if the DTL will be instrumented. As far as possible BPMs will be physically attached to the magnets, since the goal of beam steering normally is to centre the beam in the quadrupoles. For case of the hybrid cryomodule with cold magnets, this means that BPMs in the cold linac will be cryogenic, and integrated in the cryomodule. Processing will be narrow band, with a bandwidth of about 1 MHz. To avoid pick-up of parasitic RF signals, the BPMs will not operate at the same frequency as the cavities. In the first part of the linac, the processing frequency will be the second harmonic of the bunch frequency, while in the elliptical cavity section, where the RF frequency goes up by a factor two, processing will be done at the bunch repetition frequency.

Narrow band processing requires special care at the low energy end of the linac, since the sensitivity for a given frequency is not only given by the geometry of the pick-up, but also is a function of the relativistic beta. The BPM system will also provide the time of arrival (phase) information as well as an intensity reading⁴ at each BPM. To the extent possible, readout hardware will be shared between the BPM and LLRF systems, since requirements are very similar.

4.11.4 Transverse profile and halo

Transverse profile measurement poses a challenge, particularly in the cold linac. There are concerns that fragments from physical wires, if broken, could contaminate he superconducting cavities. However, calculations indicate that both Carbon and Tungsten wires would survive beam pulses of about 100 μ s. Carbon wires are contra-indicated by a test made at GANIL, where the effect of sublimating different wire materials near superconducting cavities was studied. Tungsten, seems to be an acceptable material, as also is Niobium. Tungsten wires would likely suffer from thermionic emission even with a short ESS beam pulse. Hence, profiles would likely need to be measured by sampling the downstream beam loss rather than the secondary emission current in the wire. Further studies are required to understand the possible geometrical effects due to the limited space, as this is known to be an issue at low gamma values.

Non-interceptive methods for measuring beam size, such as beam induced rest gas florescence or ionisation, are being investigated in parallel. These methods could allow on-line measurements of the beam size, since these methods would not require the use of a dedicated diagnostics pulse. However, they are often not considered as reliable as wire scanners, so a wire scanner may be retained for cross calibration even if such devices are installed. Carbon wire scanners – and in some cases SEM grids or harps – will be used in the warm linac. Options to measure halo include wire scanners at high gain (possibly in single counting mode), instrumented scrapers and vibrating wires.

4.11.5 Longitudinal bunch shape

Bunches in the ESS linac are very short (10 - 40 ps), and therefore options to measure the bunch length are limited. Wall current monitors (or any other method based on detecting the fields at the vacuum chamber boundary) have an intrinsic resolution limit that is significantly larger than the bunch length, due to the relatively low relativistic beta. A Feschenko-type bunch shape monitor (BSM) seems to be the best option. Such a detector is based on measuring secondary electrons from a wire placed in the tail of the beam distribution. Since the process of electron emission does not have a significant delay, very high time resolution can in principle be achieved in this way. Variants of the Feschenko monitor without a physical wire have been developed at GSI and ANL, and these are interesting options for ESS. The possibility of using the BSMs as wire scanners is also being investigated. However, it is likely that thermionic emission will blind the BSM detectors if the wire is placed in the beam core.

4.11.6 Target spot size

The SNS spot size is measured using a scintillating material deposited on the target nose, via an optical readout system. A similar solution is being pursued for the ESS, and other options are being investigated. It may be possible to avoid the restriction of using a fibre bundle to bring out the image (as at SNS) by integrating the design of the spot measurement system into the design of the target shielding monolith from the beginning. The beam spot could be measured in one or more of three positions:

1. On the proton beam window. Optical Transition Radiation (OTR) techniques, or a dedicated screen, could be used instead of a scintillator.

 $^{^{4}}$ This intensity reading will not be total bunch intensity, but the magnitude of the first or second Fourier component, so it will depend on bunch length

- 2. At a dedicated screen in front of the target.
- 3. On the target itself. Horizontal measurement appears difficult, because the target is a solid rotating wheel.

4.11.7 Front end diagnostics and commissioning

The front end will have several specialised diagnostic devices such as slits and Faraday cups. There is limited space for diagnostics in the front-end, and so the use of a temporary movable diagnostic bench is foreseen, during linac construction and commissioning. It may be possible to reuse parts of the Linac4 diagnostics bench, if it becomes available, because of the similarities between the two front-ends and the relative timing of the two projects. Commissioning scenarios, including diagnostics specifications for commissioning with low intensity beam, are being developed.

4.12 Upgradeability

The obvious advantage of a linac is that beam passes only once through the accelerating structures, enabling it to accelerate a high current beam with a minimum of constraints. The current limit is mainly set by space charge effects at low energy, as well as by the power that can be delivered to the beam in each accelerating cavity at medium and high energies, and by beam losses. The ESS accelerator high level requirements are shown in Table 2.

General considerations. All upgrades beyond the original design goals will require a redesign of the target for cooling, shielding, and/or the possible addition of a new target station. The macroscopic time structure of the proton beam at a pulsed spallation source is intimately linked to instrument design and location.

The spallation cross section for protons on heavy nuclei increases as a function of proton energy up to several tens of GeV [108]. Nonetheless it is generally agreed that a kinetic proton energy between 1–3.5 GeV is optimal for practical target and moderator designs, and in order to keep the shielding requirements reasonable. An upgrade based on an energy upgrade must consider this limitation and also take into account the change of target conditions at higher energies for example the peak of neutron production for the proton beam will move by a few centimetres for an energy increase from 2.5 to 3.5 GeV. This will influence the efficiency of the neutron moderators and possibly increase the number of protons scattered around and through the target. However, a pure energy upgrade using additional accelerating structures will have little influence on beam dynamics and will not require any major modification of the existing lattice.

Increasing the current of the proton beam will require more RF power to the beam, and will require a redesign of the front end, including the ion source, and of the RF sources for all accelerating structures. Since space charge increases, and the matching between RF sources and the accelerating structures will change, it is also likely to require a change of the accelerating structures, and of both the primary RF couplers and possible HOM couplers. For extreme cases it might be necessary to have two front-ends, allowing the beams to be funnelled together at a higher energy when space charge is less of an issue. It will also have an overall impact on beam dynamics. Preliminary studies suggest that the present solution with a single front-end operating at 352 MHz could be designed for up to 100 mA average beam pulse current.

Increasing the repetition rate or the pulse length will require will require new RF sources but will have little or no impact on beam dynamics and SCRF. However, it will require new instruments or a redesign and possible relocation of existing instruments. A possible away around this is to add a second target station, to which (for example) the additional pulses are extracted or part of the pulse is deviated.

4.12.1 Scenarios

The linac design is gradient-limited rather than power-limited, implying that the beam energy cannot be increased without adding cryomodules. However, the linac is close to being power-limited, with the power couplers for the elliptical cavities being specified for 900 kW. This is just beyond the \sim 850 kW of power that is required to be transmitted to the beam per cavity in the high beta section of the current linac optics [82]. The RF sources are foreseen to match this power requirement and will be able to deliver 900 kW with a modest margin in the high beta section [109]. The linac is more strongly gradient-limited in the spoke resonator and medium beta elliptical sections, where the power to the beam per cavity is lower.

Energy upgrade. The present linac layout includes 100 m of space in the HEBT that is available for upgrades. It would be straightforward to increase the energy to 3.5 GeV by adding 8 cryomodules of the kind already used at the end of the linac. Such an addition would fill up the available space, delivering 7 MW of beam power. The downstream end of the HEBT, including the vertical chicane up to the target level, is designed for 3.5 GeV operation, to prepare for this upgrade scenario.

Current upgrade. Instead of going to 3.5 GeV as a first step, the beam current could be increased to, say, 100 mA. This would require 5 additional cryomodules if the power couplers remain limited to 900 kW, since the high beta section would be power-limited, and the accelerating gradient there would have to be reduced. The power per cavity would have to increase in the other sections, to keep the speed gain compatible with the cavity geometric betas. Thus new RF sources would be needed for these sections, making this option less attractive for a minor power upgrade. Increasing the current to 100 mA or higher also requires an ion source that is more powerful than the one initially foreseen, although the RFQ will be designed for 100 mA. The DTL may need to be designed with stronger quadrupoles for 75 mA or 100 mA operation.

At present the linac optics – geometrical betas, number of cryomodules per section, et cetera – is designed for 50 mA. Alternatively, it could be designed for a higher current, in which case fewer cryomodules (perhaps only one for 7 MW) and fewer power sources would be needed for an upgrade. This would save costs, but there would be initial disadvantages, for example in having geometrical betas further from their optimum values because of increased power in the passband modes. Similarly, coupling the power to the beam would become less optimal, unless the power couplers could be made adjustable.

Energy and current upgrade. A major beam power upgrade – to more than 7 MW or 8 MW – needs a combination of higher energy and higher current. Figure 59 indicates that an extreme scenario, going to 100 mA with 3.5 GeV for a power of 14 MW, requires spoke resonator power couplers rated at 500 kW, and elliptical high beta cavity couplers rated at 1800 kW. Two couplers per cavity could possibly be used in the high beta section. The power in the the medium beta section would reach 1.1 MW per cavity at 100 mA, more or less within reach of the nominally 900 kW couplers. If absolutely necessary the medium beta power per cavity could be reduced by adding an extra medium beta cryomodule in the 50 mA baseline design. Although both alternatives require some extra R&D, they could probably be included from day-one without significantly increasing the total cost of the cryomodules.

4.12.2 Superconducting RF

RF power sources. The major cost for any major power upgrade would clearly be the RF sources. If they are initially dimensioned for the baseline 5 MW linac – and anything more would come with a significantly increased initial cost – a substantial upgrade would require more or less all sources to be replaced. As a possible alternative, the old sources could be re-used by having two klystrons per cavity in part of the linac. However, this has the disadvantage of taking even more space in the klystron gallery, which is already large even in the 5 MW baseline with a single klystron per cavity, with an unprecedented amount of RF equipment to be installed with less than 2 m on average between the accelerating structures. A possible way forward would be to initially supply more than one accelerating structure from each RF source at twice the nominal power, leaving space for additional sources to be installed later. Alternatively, enough space must be left for a second RF gallery and associated wave guides. Two RF sources powering two different couplers on the same cavity would require that the RF sources are identical or that one RF source is split perfectly, otherwise significant power bleeds from one system to the other.

Power couplers. Power couplers are typically matched to a certain beam current so that the power reflected from the cavity is minimised by the term related to the beam loading. An increase in beam current in the cavity by 50% would increase the loading, resulting in an increase in the reflected power. An initial estimate suggests that this increase would be 4% of the power arriving at the coupler. This impact could be reduced by matching the coupler to an intermediate beam current, trading off a marginal increase in the reflected power (with nominal beam current) for a reduction in the impact of the upgrade. An initial configuration with two couplers per accelerating structure would require that both couplers are used from the beginning. If not, the second coupler would absorb a lot of power (if resistively terminated) or would shift the cavity modes significantly (if reactively terminated), most likely causing large standing waves inside the idle coupler. It appears to be easier to over-design a single coupler for high power from the start – for example, 1.8 MW for the ESS high beta elliptical section.

Higher Order Modes. Any increase in beam current will cause a quadratic increase in the HOM power, and so will strongly increase the risk of these parasitic fields having negative effects on the operation of the machine. Therefore, such an upgrade path adds considerable weight in favour of the decision to install HOM couplers as a part of the baseline.

4.12.3 Discussion

Higher power operation can be envisaged. Preliminary studies suggests that the beam energy can be upgraded to 3.5 GeV within the existing target design and layout, and that the linac could be prepared for a beam current increase to as much as 100 mA. Sufficient space must be left empty in the tunnel for additional cryomodules, to preserve the energy upgrade option. Further detailed studies will set the path and the limits for possible upgrades. However, it is clear that major savings and flexibility can be gained from wise baseline design choices.

5 Control Systems

5.1 Design

Integrated Control System organisation. The Integrated Control System is a sophisticated combination of software and hardware connecting all the various parts of the ESS machine and is essential for the synchronisation and day to day running of all equipment. Its organisation will inevitably also determine its efficiency and usability. A certain degree of flexibility is expected. The ESS machine consists of four major parts that make use of the Integrated Control System :

- 1. Accelerator, which in turn consists of several sub-systems.
- 2. **Target** which in this context consists of measurement of target parameters during operation, such as temperatures, flow rates, beam footprint.
- 3. Instruments, which in this context consists of the scientific instruments including neutron beamlines and the sample environment. Experimental data acquisition, storage and analysis is discussed in a separate Chapter.
- 4. **Conventional facilities**, which consists of the air conditioning system, cooling water, high voltage, et cetera.



Figure 105: Control System Architecture: Core Systems, Control Box, HMI, BLED and Development Environment

In order to make the control system as effective as possible and to minimise duplication, a division in terms of basic blocks from the controls perspective is more suitable as shown in Figure 105.

- 1. Control System Core This includes computer services that need to run continuously irrespective of user activities, for example, the archiving of process variable (PV) values, monitoring of alarm states and slow feedback loops. It also includes the central systems such as timing, machine protection services, et cetera.
- 2. Control Box It is responsible for interaction with equipment and devices. It serves two purposes: to provide an abstract representation of equipment to higher layers through which the equipment can be monitored and controlled, and to implement real-time control loops.
- 3. HMI (Human Machine Interface) These are graphical and non-graphical user interfaces, but also the control room as a whole. Site-wide monitoring of the ESS status, and remote access are also included.
- 4. **BLED** This is a common name for a selection of data management tools and databases used for the storage of all the relevant information regarding the machine.
- 5. **Development Environment** These are vital services that allow for proper development procedures, artefact sharing, code storage, et cetera. It also enables the upgrades to be performed to the control system software.

The Integrated Control System can also be viewed as having a three-tier architecture, as shown in Figure 106 [110]. Each of the three tiers is run physically on separate computers:



Figure 106: The three-tier architecture of the ESS control system. Upper layer: User interface. Middle layer: Processing, data management and configuration storage. Bottom layer: Equipment and measurement acquisition.

- 1. The computers of the **HMI** tier focus on ergonomics and usability. Examples: Apple iMac, Microsoft Windows or a Linux distribution optimised for desktop use (for example, Gnome or KDE user interface).
- 2. The computers of the **CS Core** tier offer high CPU performance, reliability and, depending on purpose, have access to substantial storage capacities. Examples are HP ProLiant, Dell PowerEdge, et cetera. Linux will be used as the operating system of this tier.
- 3. The computers of the **Control Box** tier have a wide assortment of different input/output capabilities. The platform would likely be modular to allow various types of input/output through field buses and custom-developed hardware. Examples: PCI, National Instruments PXI, ATCA, VME et cetera.

Control system core. The heart of the Control System is represented by a communication layer depicted by the bar and connecting lines in Figure 106. The technical term for the software that mediates the communication is middleware. The communication layer is responsible for transferring information (settings, commands, time, et cetera) between the different tiers and systems. Timing, Machine protection Systems (MPS) and Personnel Protection System (PPS) will be covered in separate sections. What follows is a brief description of software frameworks used for middleware and a list of Control System services and networks.

5.1.1 Software frameworks

A software framework, in computer programming, is an abstraction in which common code providing generic functionality can be selectively overridden or specialised by user code providing specific functionality. Frameworks are a special case of software libraries in that they are reusable abstractions of code wrapped in a well-defined Application Programming Interface (API), yet they contain some key distinguishing features that separate them from normal libraries. Software frameworks will be used, as they address non-functional requirements, such as scalability, look and feel of the graphical user interface, communication among distributed processes, et cetera. By leveraging a framework, the developers of control system applications can focus their efficiency. Selecting a proper framework for all tiers and verticals is not straightforward, because on the one hand, no single framework provides an optimal solution for all tiers and verticals, which in turn would suggest that a mixture of framework results in both lower development as well as operational costs and fewer spare parts need to be maintained. Thus, we seek the best compromise between the choice of framework and functionality on the one hand, and standardisation on the other.

The EPICS control system framework will be used for Control system Core and Control box software. EPICS is widely used at many large physics facilities for system control including proton accelerators at neutron sources (SNS and J-PARC) and electron accelerators as well as instrumentation for synchrotrons (DLS and SLS). EPICS is supported by a very large community with two annual collaboration meetings and an annual technical meeting. Consequently, EPICS drivers already exist for many devices including those used by many Instruments. Moreover, EPICS is also used by ITER and as mentioned earlier, by SNS. These two facilities are based on contributions from geographically separated laboratories and have made or are making use of the Control Box methodology of structuring the development. The middleware in EPICS is called Channel Access.

EPICS interfaces to the real world with Input Output Controllers (IOCs) which are standard PCs, VME, PCI, ATCA, et cetera or standard embedded system processors that manage a variety of "plug and play" modules (GPIB, RS-232, IP Carrier et cetera) that interface to control system instruments (oscilloscopes, network analysers) and devices (motors, thermocouples, switches, modulators, power supplies, et cetera).

EPICS is not yet used widely for instrument control at neutron facilities. The SNS faced similar issues during its construction as the ESS will face, namely coordinating different laboratories and their efforts to build ESS specific neutron scattering instruments. SNS is gradually overhauling their systems to have a unified control system for not only the existing Accelerator/Target control system but also the neutron scattering instruments. Standardising early in the project will benefit ESS in the long term. Potential development for ESS instrument specific EPICS drivers could be done in close collaboration with other labs using similar equipment.

5.1.2 Control system services

There will be several services running automatically, independent of the operator control.

1. Alarm system. The alarm system is a messaging system: it collects, manages and distributes information about abnormal situations and displays this information to the user. In a complex environment, a malfunction, either in the software or the hardware, might trigger a chain of malfunctions in other equipment. The main purpose of the alarm system is to help the user identify the root cause of a problem in such a way that he can fix the problem in a short time. This is achieved by comparing the alarms active at a given time against a knowledge base describing the correlation between the alarms.

- 2. Archiving and post-mortem services. Archiving provides the mechanism to store machine configuration and readback data to a permanent location. Archiving consists of:
 - (a) Trending: archiving of variables over time. Trending is performed at a slower data rate than live display of data. It is not done for control purposes, and it is stored in permanent storage.
 - (b) Post-mortem storage: Post-mortem can be triggered on: request, emergency (for example interlock signal of the MPS), a timing event, a network event (by adding accelerator context information, post-mortem data can be correlated later).
 - (c) Archiving service: The archiving service stores historical values of properties in the control system. Archiving can be configured on a per-property basis, and can be done either on-time (archiving of a value at a certain frequency), or on-change (archiving of a value as soon as is it changes for a pre-defined amount).
- 3. Logging service. Central logging service collects log entries from throughout the system. Log entries are best stored in a relational database to allow for efficient querying. The purpose of logging and error systems is to allow operators and control system maintenance team to quickly pinpoint the root cause of a failure and resolve it in the shortest period of time.
- 4. Gateway. The Gateway is both a Channel Access Server and Channel Access Client that provides a means for many clients to access a process variable while making only one connection to the server that owns the process variable. It also provides additional access security beyond that on the server. It thus protects critical servers while providing possibly restricted access to needed process variables. The Gateway typically runs on a machine with multiple network cards, and the clients and the server may be on different subnets.
- 5. Save and restore. It should be possible to create a snapshot of a subset of selected controls variables, part of a database (a well-defined collection of records) or an individual record. Later, it should be possible to retrieve a particular snapshot, and merge it with another snapshot.
- 6. Video network. Video service is based on bulk data transfer service, and is specialised to deliver video streams. Video streams are typically delivered using protocols running on top of UDP.

Computer networks. The Integrated Control System will need several dedicated computer networks.

- 1. Control Network used by Channel Access.
- 2. Timing Network used for time synchronisation and time stamping
- 3. MPS Network used for MPS specific events
- 4. **PLC Network** used for PLC communication
- 5. Video Network used for video streaming

Each network will have to satisfy the requirements for data transfer rates depending on the needs of the related system.

5.2 Timing and synchronisation

The role of the timing system is to synchronise receiver devices, placed all around the ESS, and to perform device specific actions just in time relative to the passage of the beam. This is orchestrated by means of distributing timing-system events to all timing receivers. Master clock generation is in the domain of the Low Level RF group, and is then propagated to accelerator, target and experiment systems. The master clock drives the injector, all LLRF clocks, and all injector and linac instrumentation beam-synchronous triggers and the devices of target, beamlines and experiments that need to be synchronised to the beam. This clock is by definition beam- and RF-synchronous, and will be a multiple of the design 704 MHz primary superconducting RF frequency. Figure 107 illustrates the complex interconnections between different systems and the role of the timing system.



Figure 107: A modern timing system solution.

The most important parameters defining the timing system solution are:

- 1. Number of timing receivers; this is important for estimating total cost of ownership for the timing-system solution. Additionally, the distribution infrastructure has to be taken into account when developing accuracy and jitter requirements.
- 2. Accuracy and jitter; the timing distribution layer is to a great extent defined with these parameters.
- 3. Patterns and decision-rules complexity level for actions that must happen in real time; this will define the complexity of the timing master. The following questions have to be answered:
 - (a) Power electronics requirements; how to link the operation of the accelerator with the line frequency and possibly with mechanical choppers?
 - (b) Which real-time decisions have to be made, based on the present status of the machine and all inputs? How are alternate scenarios (pre)defined?
 - (c) How should the patterns of machine behaviour be generated on the micro and macro levels?
 - (d) What real-time data has to be collected, processed and distributed? (GPS time, machine protection system status, et cetera.)
5.2.1 Timing system architecture

Figure 108 illustrates a modern generic timing system solution. Any crate can be used, but the one used should support a variety of processors and extension cards. Micro Research Finland (MRF) is one possible transport layer. It is available in VME and cPCI form factors [111, 112]. Backplane bandwidth is practically not an issue since data throughput is relatively low because the timing master FPGA handles all real-time requirements.

Processor; control system integration. The processor board provides the integration of the timing master into the control system. Statically prescheduled machine behaviour is first loaded into processor memory. The processor then handles all required chunking and provides just in-time instructions to the FPGA for real-time execution. The processor board also provides control system readbacks to evaluate the timing system operational status.

FPGA board; timing system master real-time controller. The FPGA is required for real-time orchestration of the complete machine. For the sake of simplicity one can perceive the timing master as a collection of programmable counters sending out timing events precisely correlated to each other and external conditions (also configured for hard real-time responses). This FPGA is responsible for linking the operation of the accelerator with mains (general-purpose alternating current (AC) electric power supply), for real-time decisions based on the present status of the machine and all inputs, for generating patterns, for real-time data collecting, processing and distribution.

Event network; real-time distribution. After the timing system master generates events, a real-time distribution layer handles the precise delivery of timing signals. This layer handles connectivity architecture (to connect many receivers to a single master), as well as encoding and decoding. This layer must operate synchronously so all receivers respond to timing events synchronously as well.

Prototyping. A prototype implementation with a processor board (with Linux or RTEMS) and EPICS will help to establish the ESS scheduling needs and thus the FPGA size requirements, which will guide further development. We will consider developing a custom timing master generator, based on FPGA, using a commercial off-the-shelf solution for the transport layer and timing receivers.



Figure 108: Timing system architecture.

Timing system transfer layer concepts. There are two main timing system concepts, that to some extent define the hardware:

1. Fully deterministic data traffic.

In this case the time of sending and the time of receiving the data are fully deterministic and consequently so are the processing of such data and the corresponding actions.

Pros: simple and raw implementation, robust (one way), 15 ps jitter.

Cons: tricky automatic delay compensation, complicated slave to master communication.

2. Absolute time mechanisms.

This alternative approach uses the protocols for agreeing on absolute time, for example PTP. White Rabbit is a potential solution for this approach. The logic is more complex than the fully deterministic approach because first, the travel time of each package must be determined and second, actions can be only scheduled at some time in the future.

Pros: possible multiple transmitters and automatic delay compensation.

Cons: inherently slower master, slave communication and no implementation currently available for testing.

Hardware for timing and synchronisation. During the early design stages it can be decided through iterative collaboration with different groups what equipment to use. Also the teams should agree on the standards, for example IEEE-1588. Buying equipment off-the-shelf should be considered – a timing system based on either MRF or on Open Hardware (White Rabbit) is feasible.

Timing system requirements gathering. The process of gathering the timing system requirements starts early in the design phase, continuously iterating the list of requirements with different groups (LLRF, Beam diagnostics, Target, et cetera) on a regular basis. This will lower the possible drift in requirements (and interpretations) between different involved entities.

5.3 Machine Protection System

Under error conditions the beam could damage accelerator or target components, as well as the beam pipe itself. This could lead to high costs and long downtimes (several weeks or even months). Some of the most important potential costs are:

- 1. downtime (no experiments being performed)
- 2. equipment (replacing damaged components)
- 3. repair (time, engineers)

The basic principle of the machine protection system (MPS) is simple: observe signals on input interfaces and switch off the beam upon detection of an alarm or fault signal, by triggering one or more output interfaces and the connected mitigation devices. Further, the MPS will:

- 1. support all different phases and modes of machine operation
- 2. help with post-mortem analysis and provide controlled machine re-run
- 3. maximise machine availability time (prevent almost all false trips while not missing any real faults)
- 4. provide physicists with tools that make MPS a friend and not a time-consuming monster

Response time components. Many control devices contain information about the health of the beam or the machine. Connecting all such devices into a dedicated fail-safe network forms a system that is capable of determining whether the beam is going out of control, and reacting in time. On the other hand there are devices that can switch off the beam (or at least reduce its power) in a very short time. Reliable and timely triggering of such devices prevents damage and minimises downtime. Response time is composed of four components, as shown in Figure 109:

- 1. Time for the device to detect a failure and to inform MPS (including transmission delays), t1
- 2. Time for MPS to identify the right mitigation action(s) and to distribute the signal to appropriate output(s) (MPS can have a large network and signal propagation can be the main contributor to MPS delay), t_2
- 3. Time for a mitigation device to receive a signal and execute the mitigation action (including cable delay), t3
- 4. Time for beam already in the pipe

The total ESS response time is a few microseconds. Only part of this is available for MPS devices and for the interconnecting network.



Figure 109: A graphical representation of response time composition

Support of machine construction and different modes of operation. To support all phases and modes of machine operation MPS will:

- 1. Provide support for commissioning: the machine is built step-by-step. When some segment of the machine is completed, it can be commissioned and therefore MPS should already be available. MPS will allow running only a partially built machine and will support different commissioning scenarios. MPS will grow with the machine.
- 2. Adapt its operation and protection logic to chosen machine operation: the accelerator will support various machine modes (such as the location of the beam trajectory) and beam modes (type, pulse length, power of the beam). MPS will adapt its operation for each such machine operation mode. MPS adapts its operation by changing protection logic (response matrix) and by masking (bypassing) irrelevant input signals.

Masking or bypassing MPS input devices provides great flexibility to an operator. It can be used not only for adapting the MPS to machine operation but also in many other situations, for example, when there is an unstable device preventing the machine to run, or when there is a broken device that needs to be replaced. If such devices are not critical, meaning that the machine can run safely without them, they can be (temporarily) masked.

Post-mortem and controlled machine restart. MPS will provide the evidence of a fault by logging input device changes to provide a baseline for analysing what went wrong after a trip occurs. Logged changes will be equipped with a precise timestamp and will be time synchronised so that they can be merged into a common timeline. Other, non-MPS devices that are logging signal changes will all be synchronised to the same synchronisation source – the timing system. Post-mortem analysis will be performed and the real causes will be established. If necessary, the causes will be removed before the next run. Procedures for the machine restart will also be put in place. Different restart procedures can be enforced according to the severity of a fault. If there is a minor fault, the machine can restart immediately, even automatically. For major faults, we will define which steps and measures must be taken before the machine is allowed to restart. Machine restart is an action granted only to authorised personnel.

Maximising availability. A reliable MPS will respond on each detected alarm/fault. No faults should be missed! On the other hand, a reliable MPS will minimise false trips and consequently maximise machine availability time. The final success depends on the reliability of the devices connected to the MPS. The following measures will be taken to improve reliability:

- 1. Failsafe design. Any MPS failure will be detected and the machine/beam will be preventively stopped. All devices connected to MPS will be failsafe designed as well, so that their failure always leads to a safe machine stop.
- 2. Critical component redundancy. Redundancy will be applied at many levels. The most important is to have redundant mitigation devices so that stopping the machine will never fail. Other redundancy such as duplicated interconnections or redundant devices is also possible.
- 3. Operators will have a tool to diagnose inputs (that is devices connected to MPS). Any unstable device, which is not critical for machine operation, can be masked to prevent false trips.
- 4. Self-diagnostic procedures to verify MPS health. The machine will be safely stopped if any malfunction is detected. Other procedures could be implemented to verify MPS configuration before machine start-up.

MPS requirement gathering. The process of gathering the MPS requirements starts early in the design phase, continuously iterating the list of requirements with different groups (Beam diagnostics, Target, et cetera) on a regular basis. Such an approach lowers the possible drift in MPS requirements (and interpretations) between different involved entities.

5.4 Personnel Protection System

The main concern of the Personnel Protection System (PPS) is to preserve the safety of personnel and the public. It adheres to nuclear safety and all other relevant safety regulations. It includes a Personnel Access Safety System (PASS) and a series of safety interlocks to prevent the beam operation in the event that persons inadvertently enter an unsafe area. The PPS and PASS systems will be highly redundant. Two teams will be independently engaged in developing and deploying independent systems that individually meet all the requirements of PPS.

The level of responsibility for the PPS in the domain of the Integrated Control System department has not yet been determined. However, most of the responsibility for personnel safety lies within the Health, Safety and Environment group.

5.5 The Control Box

Because the development of the machine will be geographically and organisationally distributed to many laboratories, it is important that a controlled way of developing the control software is implemented that enforces a high level of standardisation. Therefore the Control Box methodology is adopted, based on the development philosophy established by SNS, a spallation source that was built in a similar collaboration as ESS. The same approach was taken further at ITER, a project that faces the same distributed organisational challenges. The Control Box is simply a server that controls a collection of devices, for example an instrument. In ITER terminology, the Control Box philosophy is realised with the concepts Plant System Host, CODAC, mini-CODAC and plant system I&C [113]. To make the complete control system, these servers simply need to be interfaced to the middleware so that they can communicate with the HMI and CS Core central services.

Control Box architecture. EPICS will be used as the software framework for control systems. EPICS is a software framework for control systems that comes with middleware in the form of a Channel Access (CA) layer, drivers for interfacing the hardware, and distributed Input/Output Controllers (IOC) associated with specific devices. These devices know how to convert input signals to meaningful data as well as make software commands understandable by the hardware devices. Because of this feature, an IOC with associated drivers and corresponding CA layer translates directly to a Control Box. An example of an EPICS based Control Box is shown in Figure 110.



Figure 110: A schematic example of typical Control Box components. The Control Box hardware and software are composed of two main logical parts: services and operator interfaces, and device control with an EPICS IOC.

The main purposes of the Control Box are to:

- 1. Allow independent and yet standardised subsystem controls development,
- 2. Encourage and enforce consistency between sub-systems (including target and experimental stations),
- 3. Facilitate new component testing (for example EPICS drivers),
- 4. Allow factory acceptance testing of subsystems through the control system,
- 5. Validate technology decisions,
- 6. Mediate early risk reduction, to prevent unexpected surprises at project integration time,
- 7. Force the controls group to make and document early decisions,
- 8. Minimise throw-away hardware and software development

The hardware in a generic Control Box based on EPICS consists of one or more input/output controller (IOC) computers, and zero or more I/O modules (analog-digital converters and digitisers, digital-analog converters, serial interfaces, et cetera.) attached to the IOC computers hardware bus. The software in a Control Box includes:

- 1. A real-time or non-real-time operating system, depending on requirements on IOC processing. For example, IOC real-time control loops require an IOC real-time operating system.
- 2. The EPICS real-time database maintains the values of all process variables under responsibility of the IOC.
- 3. EPICS device support, which implements drivers for communication with equipment.
- 4. EPICS Channel Access, which allows the process variables on the Control Box to be accessed from other computers in the network, and can retrieve values of process variables from other IOCs.
- 5. PLC subsystems for slow industrial controls (for example, water cooling, HVAC, et cetera) are connected to the IOC with one of several standard communication mechanisms, such as PROFINET or Modbus TCP/IP. An Ethernet-based bus permits the same kind of cabling and switching equipment that is used for other networks to also be used for PLCs. This makes the PLC network easier to connect to the IOC, as a regular network interface card and associated drivers are used instead of a special-purpose PLC bus adapter.
- 6. Control of a large number of PLC devices may require an Ethernet switch.
- 7. A separate network will be used for PLCs, so that the PLC network traffic is predictable. Otherwise, network traffic could interfere with operation of the PLCs, which in some cases are safety-critical.
- 8. Intelligent special-purpose controllers (for example, possibly LLRF controllers).

Specifications for the layouts and structures of ESS Control Boxes will be informed by the different possible structures specified and documented for ITER [114].

Control Box development. The Control Box will not be completely defined and developed too early in the project, because the supporting technology landscape is rapidly evolving. Iterative development will be pursued for Control Box software and hardware, in yearly cycles. This starts with software-only aspects (the easiest to develop, test and distribute) delivering a Control Box with a simple standardised hardware interface, such as infrastructure PLC control, as soon as possible. Increasing functionality will be added later, including hardware support, timing and feed-forward systems, as tools and support evolve with available technology and resources.

5.5.1 Equipment interface

The control system will be partitioned into separate subsystems that are closed entities and can be assigned to one supplier, such as to an internal team, to a collaborating institute or to a commercial vendor (for example, for the vacuum or cryogenic subsystems). The Control Box metaphor ensures that these systems are treated separately (for example not sharing hardware interface units). Strict guidelines for their development will be provided, enabling the clear division of responsibilities and making integration much easier, a particularly vital necessity for distributed subsystems. There are two types of equipment interface: hard real-time, and non real-time.

A hard real-time equipment interface is needed whenever the Control Box response to external events must be guaranteed. This is needed in only a minority of cases, because specialised hard real-time subsystems and intelligent special-purpose controllers already address the real-time aspects of control. For example, LLRF hardware will already close real-time control loops. Either a real-time operating system must be used on the IOC when hard real-time response is needed, or the functionality must be implemented in hardware (for example, FPGA). When a real-time interface is required, the real-time information will be distributed between subsystems only by means of the timing system. No other real-time communication will propagate between different subsystems. This isolates all aspects of subsystem real-time behaviour to those subsystems, which can then be developed and fully tested earlier in the process, during factory testing and acceptance, rather than later during site testing, acceptance, and integration.

A non real-time equipment interface has limited responsibility for making process variables and parameters of hard real-time control loops available to other subsystems and user interfaces. Some equipment has its own real-time control (for example, PLC systems, temperature regulation, motion controllers, LLRF fast control feedback loops, et cetera). Here the control system only needs to slowly control the parameters of these low-level control loops and monitor their diagnostics (for example, monitoring PLC registers, setting reference temperature, manipulating PID control loop parameters, et cetera). Some equipment needs to exhibit real-time behaviour, but can be controlled in a feed-forward manner (for example, high-level control of the superconducting RF). In this case, the control system distributes the information on what actions to take (for example, waveforms defining value of set points as a function of time), while the timing system distributes the time and event triggers.

I/O Interfaces. The number of different I/O types will be reduced to minimise the driver development and maintenance burden. A single, standard bus architecture with standardised I/O modules will be selected. Examples of I/O modules include:

- 1. Time receiver module for providing synchronised time across the entire facility for time-stamping of acquired values and synchronising time-critical activities.
- 2. Ethernet for main control system integration and interfacing of network attached devices (interfacing also serial or GPIB devices and instruments via RS-232 or GPIB to Ethernet converters). This also includes read-only interfaces to safety and machine protection systems
- 3. Analog and digital I/O, for example for power supply read back.
- 4. Digitisers of various sample rates and precision, for example digital oscilloscopes, spectrum analysers, and other high-bandwidth devices.

5.5.2 Hardware platforms

There are three main candidates for a general control system IOC platform: VME, ATCA, PCI and their derivatives. A choice will be made after considering their principal characteristics according to the most important properties, which are:

- 1. Vendor support: how many commercial vendors of crates and modules exist? A large number implies a higher probability of finding an off-the-shelf module for a particular task.
- 2. Maturity: how long has the platform been available and how frequently is it used? Greater maturity implies lower risk and lower probability of backward-incompatible changes in the future.
- 3. Longevity: how long is the platform expected to be available? Assessment will consider the (several decade) ESS lifetime.
- 4. Maximum transfer rate: how much data can the platform transport between the modules in a given time? Measure both throughput and latency.

- 5. **Topology**: how can the modules interact with each other? For example, slaves in a master-slave topology do not directly interact with each other.
- 6. Form factor: how large is the physical size of a module in a rack? Larger form factor allows more I/O points on the module, but also increases the amount of rack space that is unused for non-I/O modules.
- 7. **High availability**: how suitable is the platform for high-availability applications? Is there support for redundancy?
- 8. **Software support**: how likely will software support (Linux driver, EPICS device support) be available for a module?
- 9. Cost: ranking relative to the cost of the crate and modules.
- 10. Users: How many accelerator, target, protection system, and instrument controls groups or facilities have adopted the platform?

5.6 Control equipment catalogue

In the early design and prototype stages it is important that a certain level of agreement on HW components and platforms between different groups is achieved. The controls group proposes the ITER approach to tackle the complex equipment discussion to simplify the integration of groups and their equipment in the control system. Such an approach should cover the following steps:

- 1. Study of available components and iterative meetings with the users (groups) to find the proper solutions / components for both parties involved
- 2. Full support of the HW component by the controls group and the integration into the control system (by using the Control Box and the Development environment)
- 3. Adding the fully supported component to the catalogue thus making it available to all possible future users
- 4. Providing support and further developments for the listed components

Such an approach facilitates integration of single components, various prototypes and production hardware into the control system. Also, with such an approach the integration effort during the construction and operation phase will be significantly lowered because of the unified components and support. The catalogue will provide a full list of equipment that is approved for use in the control system for example make and model (for example, NI-6682 timing card). In cases such specifics are too restrictive at least the standard (for example, IEEE-1588) should be listed.

Control boxes for complex subsystems. The distribution of control boxes will be optimised between performance, complexity, and cost. In the simplest case, when equipment is close, the control box can be directly connected to subsystem equipment with signal cables. Examples might include the ion source and the proton beam choppers, located at the front end of the linac, and each of the scientific instruments. A single control box will be sufficient for many one-of-a-kind subsystems. In a more complex case, the equipment covers a wider geographical area, and is more numerous. For example, the numerous superconducting cavities, with their associated klystrons and cryomodules, will be spread along most of the linac. In this case it is impractical to control a complete subsystem with a single control box. One control box for each type of equipment will be placed at periodic intervals along the length of the linac.

5.7 BLED

Configuration data management. The data needed for the operation of the ESS Control system will be centrally managed. This system has been named BLED. It will take the form of one or several databases and will include several tools and utilities for database management. BLED will be tightly connected with the development environment and will present a natural gateway for the introduction of new configurations of the control system. This all-encompassing approach will include the information on the location of the equipment; it will also include the data about the lattice, cabling information and various high-level configuration parameters of the facility. BLED will list all process variables, alarm definitions and alarm configurations and process variable archiving configurations. Basic information about the personnel who are making changes to the database is also included.

Implementations of BLED can be based on existing solutions used in the accelerator community, and development can be done in collaboration with other institutes, such as SNS, BNL, FRIB and ITER. Different approaches to implementation should be evaluated based on the match between ESS requirements and existing solutions. Database entities will be versioned and several instances will be available for different use cases. This will make it possible to recreate an older version of the facility machine model or even to recreate just some parts of the model. BLED will be constructed and operated so that it will provide a consistent model of the entire facility configuration.

BLED covers configuration data management from several perspectives:

Naming convention perspective. Various parts of the ESS (accelerator, target, instruments, et cetera), that will be managed by the Integrated Control System, are hierarchically structured into systems, subsystems, devices, signals and process variables. All this information is stored in BLED. The ESS Naming Convention for devices, equipment, signals and process variables leverages this hierarchy [115]. Therefore the name of a particular signal or process variable in the system is composed from the names of the system, the subsystem and the device where this signal or the process variable resides. (Here, "signal" refers to an EPICS process variable, which corresponds to a physical signal on some device in the system.) For example, the name for the command signal of the accelerator for the current (I) set point (Set) of the 10th power supply of the magnets subsystem in the first DTL tank is **DTL1-Mag:PS-010:ISet**

Parameter lists perspective. A parameter list database and web interface tools ensure consistency of the information being used amongst all subgroups that subscribe, throughout the period of ESS design and construction [116]. These tools identify inconsistencies among parameters and enable groups as well as individuals working towards the same solution. Another goal is to make the parameter lists easily accessible and useful to a wider audience. The parameter list database is relational and normalised to at least the 3NF level [117]. The parameter list can be seen as a communication tool within and between different groups and individuals in the collaboration. It is therefore natural to categorise parameters by teams, or roles within the teams. The second classification of the parameter list access is versatile, self-explanatory and efficient, using a Java based web interface tools. A certain amount of control needs to be established, for example, for units [Units], dependencies and user privileges; nevertheless this is kept to a minimum. Query tools generate parameter lists in a readable fashion, similar to the parameter lists on the ESS-AD home page [81].

Lattice perspective. Accelerator parts that belong to the lattice are characterised by additional beam optics attributes and by other device characteristics (such as bending angle, aperture size, magnetic field parameters, RF parameters, et cetera) which are needed during the design and physical construction of the linac. High level applications for beam control require this information during commissioning and operations.

Mechanical engineering perspective. Once the lattice model is designed, the lattice configuration data will be used to generate the survey configuration files, which are used for the layout of mechanical and conventional facility engineering.

Infrastructure perspective. ESS infrastructure consists of buildings and rooms where the equipment is installed. This equipment is either stand-alone or placed in racks. Configuration database models the premises and keeps track of the exact location of servers, IOC controllers and switches inside the racks, rooms and buildings. Doors, rooms, racks, et cetera are all named according to the ESS Naming Convention.

Wiring perspective. BLED stores cabling information for devices that are interconnected with cables. This is achieved by defining the types of cables, ports and connectors and by storing the actual mapping between the ports and cables.

Control system perspective. The naming perspective already provides the necessary support to identify all process variables in EPICS. Several configuration file generation tools will be needed in order to generate all EPICS database configuration files from BLED. EPICS process variable fields, alarm server configurations and channel archiving configurations are added to BLED to enable the generation of the EPICS database files, alarm configuration and channel archiving configuration. Graphical database editing tools leverage the configuration database. Schema will be extended also with diagrams and with positions of process variables on the diagrams.

Software tools perspective. Various software tools benefit from their interoperability with BLED, which is accessible in the form of a service through a Java API. Figure 111 shows the high level BLED architecture and how various types of ESS software tools use it. The Java API makes possible for some dedicated tools to use the BLED service directly. Table 45 lists ESS software tools that could be connected to BLED, and determines what types of connection need to be implemented (Java API, data import, data export, or data import and export). The type of the synchronisation is also listed below (on demand, or periodic), for tools that require data synchronisation.



Figure 111: High level BLED architecture.

Tool	Communication type	Synchronisation type
BLEDconfigurator	Java API	
Lattice design tool TraceWin	Import/export	On demand
Lattice design tool MAD	Import/export	On demand
Conventional Facility tool Survey	Export	On demand
EPICS	Import/export	On demand
XAL	Export	On demand
BEAST	Import/export	On demand
EPICS Channel Archiver	Import/export	On demand
Equipment inventory tool	Import	On demand, periodically
ESS IT User management	Import	On demand, periodically
Software deployment tool	Export	On demand
Mercurial	Import	On demand
Document management tool	Import	On demand
Wiring tool	BLED Java API	

Table 45: List of BLED-enabled ESS software tools

5.7.1 BLEDconfigurator

BLED serves its purpose only if the data it stores are up to date and synchronised with the data that are in operational use by the particular software tools. A number of measures will be designed and implemented by the tools to enable this and to enforce it where feasible. An example of technically enforced data consistency is that IOC controllers will only start if their database configuration was generated out of the central configuration database. It is mandatory that the process of configuration data modifications is hassle-free, in order for the smooth adoption of the central configuration database by all stakeholders. Thus, BLED-related software tools will provide a proper level of automation when dealing with data from BLED. In addition, working instructions and organisational measures will be put in place to enforce the proper usage of the tools to achieve the appropriate consistency of the data in BLED.

BLEDconfigurator is a Web portal that provides a graphical user interface to access BLED configuration service and databases. This portal is used by all stakeholders to perform the administrative and operational actions on the accelerator model. The portal is composed of several sections, each covering a particular set of operations. The portal provides user authentication and authorisation services to facilitate authorised use of the ESS configuration data. The portal consists of the:

- 1. Database administration section (BLEDadmin),
- 2. Model browser, manager and reporter section (BLEDmodel),
- 3. Naming-related section (BLEDnaming),
- 4. Synchronisation management section (BLEDsync),
- 5. Parameter list management section (BLEDparameters),
- 6. Lattice design and construction tools (BLEDlattice).

BLEDadmin This section of the portal combines the portal and database administrative operations like database backup and restore, database imports and exports et cetera.

BLEDmodel This tool will be used to construct the initial version of the accelerator configuration and to expand or modify it. A dedicated model browser will be provided here. In addition, BLEDmodel will be used to generate various views of the accelerator, for example an inventory list of all accelerator parts with their detailed descriptions, or hierarchical view of the systems, subsystems, devices and signals. BLEDmodel will be an important part of the Machine model.

BLEDnaming The configuration database models the envisioned ESS structure and contains actual ESS setup at a given point in time. This is exactly the information needed to implement the ESS Naming Convention tool. In fact, the BLEDmodel entities browser provides already a number of features needed by the naming tool. Therefore, it makes sense to combine the two user interfaces. The naming tool should be used as a starting point for all other accelerator design and development activities. For example, when the lattice design process for a new linac element is started, using the naming tool generates the name of the element.

BLEDsync This section provides synchronisation commands for the ESS tools that need data synchronisation with the central configuration database. Either "on demand" syncs are started by running the proper adapter or a schedule of periodic syncs is managed here. This section provides also the status of the previous syncs.

BLEDparameters This section contains operations for the management of various ESS parameter tables. ESS staff members and authorised collaborators can update the content of the parameter tables. Parameter tables can be exported in popular PC automation document formats and published to the ESS extranet. The tool shall also provide utilities to search for parameters, based on the System or owner, et cetera. Like some other control system related BLED entities, they are subject to version control.

BLEDlattice BLEDlattice is designed in a way that can supersede the DBSF tool. Lattice designers can use BLEDlattice to import the initial lattice design model from, for example, TraceWin or MAD and construct correct Control system names for them in the central configuration database. Then the lattice configuration data (with additional Control system metadata) can be generated from BLED and exported back to the TraceWin or MAD format and used for further work. When the next iteration of lattice design work is completed, the beam optics data from design tools can be imported to the BLED database by using the already defined element names for proper correlation. There may be several iterations of data exchange between the design tool and the central database before the lattice design is finished. Afterwards, data export of lattice element descriptions to the Survey format can be made.

As a side effect of the lattice design and integration process described above, a number of Control system entities will be already properly named and entered into the central configuration database. There they can be further expanded and augmented with various application specific attributes.

5.7.2 BLED tools

EPICS adapter. The EPICS IOC configuration files for the EPICS database can be generated from BLED. In order to cope with illegal changes of EPICS database files by the developer, a consistency checking tool is needed to show the differences between the generated EPICS database file and the actual one. In case that the tool finds some differences, the developer is advised to incorporate them in BLED manually. In order to improve the usability of BLED and increase the adoption of the tool by Control System developers, it would also be useful to implement the import of EPICS database configuration files in BLED and create BLED entries from them. In this process also name checking of the process variables is performed. Manual supervision of the EPICS database configuration file import process makes it possible to add the missing pieces of information and to link the process variables to the appropriate positions in the model. To simplify repetitive export/import process, EPICS database configuration files could be extended with BLED-specific pseudo commands to reduce the manual intervention steps during import. EPICS generator will deal also with control system alarm and archiving configurations and servers. They will be modelled in the configuration files.

HMI adapter. Once the lattice design is completed and imported into the central database, HMI configuration files can be generated. HMI adapter needs only the export part.

Equipment inventory database adapter. Information about the computing equipment which will be located on the ESS premises and which is entered in the ESS inventory management tool will be available from the ESS ERP system. A semi-automated import adapter for BLED could be built to import the basic data about the computing equipment and link it to the IOC and server configurations which already exists in the central database. Equipment inventory system at ESS could be also a source of the information about the exact location of particular machines in the buildings. A yearly inventory check process could provide new locations of the equipment for central database housekeeping.

Wiring tool. A wiring tool will be able to extract all the cabling information from BLED. As all the devices are already entered into BLED, only the wiring specific information must be added.

Software deployment control. Once the machine model is completely populated with the information, a dedicated software deployment tool can be used to assign and verify that correct software parts and configurations are installed on the IOC controllers and control room servers. In addition to the deployment of the latest system version it should be possible to revert to some previous version of the software and configuration for a particular device or device type in case of field errors on some particular devices. The software deployment control is also a natural delivery point for all the new software from the Development Environment.

ESS IT user management. IT user management system will be used by BLED in two ways. Firstly, user access roles to the BLED-related software will be obtained from the central ESS IT user management service. Secondly, basic user data like user names, email and roles will be imported into the central database and will be used to enrich various reports with responsible person data where appropriate.

Document management system adapter. The approval and sign off of documentation related to design, testing and other project-related documents will be managed by a dedicated application in the Project Office. In the future it will be useful to store links (URLs) to certain documents in some BLED configuration database entities. For example links to maintenance manuals for subsystem type entities or particular certification documents could be linked in the device instance entity.

Mercurial adapter. Mercurial is used as versioning system of source code and configuration files. Some entities in configuration database will include links to the particular version of the file in the Mercurial repository.

Versioning. Database Entities in BLED will be versioned. This means that it will be possible to revert to some earlier version of the entity and make it the current version for entities where this is feasible and makes sense. For example, it will be possible to revert to an earlier database configuration for a particular IOC controller or to revert to an earlier version of the entire application on all IOC controllers where it is used.

Access authorisation. BLED will be accessed by a number of tools and adapters through the Java API. It is assumed that all tools are capable of user authentication and authorisation through the central ESS IT user management infrastructure. Tools which are not capable of user authentication and authorisation should be installed only to the computer systems which belong to the people authorised for certain type of database data manipulation. There will be at least a distinction between the full BLED access rights, BLED entity creation and modification rights for the lattice designers and control system programmers, and read-only rights for other users who only need some data from BLED. During the detailed design phase it will be determined if a more fine-grained access control is needed to further distinguish between various stakeholders.

Multiple instances. The database entities in BLED should be available in several instances for different purposes. The master instance should be deployed in the production environment. For the development needs, a periodically created copy of the master instance should be available in the development environment. In addition, a developer software drop repository should include also a minimally configured copy of the central data and all related tools and adapters.

Implementation. One or more relational databases should be used for the basis of BLED. Initially MySQL should be supported. Implementation should not depend on a particular RDBMS implementation so any other type can easily replace it.

5.8 Development environment

The Integrated Control System will be complex, consisting of a multitude of subsystems that need to be integrated. Its development will require the cooperation of many developers and controls experts. Standards and guidelines will be put in place for development. Development tools and platforms will be standardised. Vital central services are being set up to allow proper development procedures, artefact sharing, code storage, et cetera, as illustrated by the graphical overview shown in Figure 112.

These services will provide the ability to:

- 1. Share artefacts (code, documents) between engineers (Mercurial, DocDB, Plone).
- 2. Perform version control (Mercurial)
- 3. Continuously integrate SW development (Hudson)
- 4. Perform complex and CPU demanding operations (DMSC)
- 5. Offer a standard development environment regardless of the platform (Virtual Machine)
- 6. Build and package software (Maven)
- 7. Deploy artefacts to user machines or IOCs (yum, rpm)
- 8. Perform automated testing (JUnit)
- 9. Report bugs and issues (Bugzilla)

The process from code development to final artefact deployment and future support will be as straight forward as possible, as illustrated in Figure 113.



Figure 112: ESS development environment map.



Figure 113: Control Box development cycle.

5.9 HMI and the user experience

5.9.1 Control room software and operator interfaces

There are significant differences between the operator interface requirements for the accelerator and target, and the requirements for the scientific instruments.

Operators. The operators for the accelerator and target are highly-trained ESS staff who are likely to be very familiar with the technical details and development of these systems and the associated software. In contrast, the typical scientific instrument operator is likely to be a visiting scientist who is at the ESS for as little as one day per year. Further, the typical scientific visitor will generally not have participated in the development of the instruments and associated software. They may come from different scientific disciplines as varied as palaeontology and physics. Users with only modest or no experience should be able to operate an instrument, and at the same time, proficient users should be able to fully exploit the capabilities of the instrument.

Development. The operator interface for the accelerator and target will be relatively complete and mature once operations begin, while the scientific instruments and associated control software will continue to evolve significantly as new instruments are added, and even after all 22 instruments are installed, responding to constant changes and improvements to meet new needs.

5.9.2 Hardware platforms for control room

Looking 10 years ahead, it seems that the smart phone and perhaps tablet PCs will be the prevalent hardware platforms for remote user control. However, the only certain prediction is that user's preferred hardware platform will change many times over the next 10–40 years. Hence, the HMI should be platform independent. One solution, in this direction, is to focus on developing a control system that functions through a cross platform web browser using a "future safe" software platform. In this way, controls developers would not have to take care of platform dependencies and would avoid the risk of having to reengineer the HMI when, in some years from now, a particular software platform is no longer supported.

5.9.3 Software frameworks

EPICS will be used for instruments drivers and communication layer of the control system. For the HMI, a number of options exist for cooperation, namely Control System Studio (CSS) originating from DESY and SNS, XAL originating from SNS, Generic Data Acquisition (GDA) originating from Diamond Light Source, and NOMAD originating from ILL that all fulfil one or more of the user requirements. By using NOMAD for instruments user interfaces, a uniform look and feel would be secured across the two European neutron sources.

5.10 Instrument and sample environment control

The instrument control system is an integrated part of the Integrated Control System. It will be synchronised with the accelerator and data acquisition control systems, and will moreover be coupled to the data analysis software so that analysed data can be used for automated control. Time stamped settings (meta data) for the instrument and sample environment will be archived so that they can be matched with detected neutrons, and ultimately enable replaying of the experiment. Indeed, the ability to match the sample to stored data set requires careful considerations with respect to design of the sample environment and associated control software, including enforcing users to make use of best practice, such as updating title and the description of the sample when the sample has been replaced.

Some of the major issues that need to be addressed by Science Division include data acquisition systems, motion control, safety interlock systems, and general automation with an emphasis on standardisation, maintainability, and compatibility between instruments and instrument control systems. Please see the chapter on the DMSC for more discussion of these issues.

A close cooperation will be established with the instrument designers, developers and associated user communities during the development phase. Moreover, standardisation will be enforced in the laboratories developing individual instruments. The control box concept plays an important role in this regard.

5.10.1 Unified user interface

The instrument and sample environment control system will look like a unified system to the user who controls the interaction between the sample condition and the instrument. However, whereas the instrument configuration is static, the sample environment varies from one experiment to the other. It therefore needs to be configured together with the static part before a new experiment. A plug and play structure is desirable, but there are situations where this is not possible, for example when a user comes with his own sample environment, or parts thereof.

5.10.2 User perspective

The instrument control system is exposed to guest scientists through the HMI that they will use to control their experiments. The requirements for the HMI are therefore challenging, because users with only little experience should be able to use it, and at the same time, proficient users should be able to fully exploit the capabilities of the instrumentation.

Instrument control user requirements:

- 1. User-friendliness. The control system should be user friendly for all users independent of background and, thus, there should be different levels of operations: simple (meaning preprogrammed common sequences of tasks) and advanced mode. A user should be able to operate the experiment based on physical/scientific terms rather than technical terms. For instance, to set the wavelength of the incoming neutrons rather than setting the chopper revolutions.
- 2. Look and feel. The same look and feel should be used for the control software for all instruments and sample environments. It is an added plus, if a user's familiarity with control software from other physics facilities, for example SNS, J-Parc, ILL or ESRF, can be transferred to ESS, meaning that the look and feel of the user interface is the same across multiple facilities. Likewise, within ESS, a uniform look and feel for all user-exposed software (instrument control and data analysis) will be an advantage both from a user perspective but also from a development point of view, because it can reduce the development burden.
- 3. Automation. It must be possible to setup batches of measurements and to define a measurement sequence before performing the actual experiment. It should also be possible to make a measurement sequence depend on the continuous status of the experiment or continuous data analysis, for instance to initiate a new measurement at a higher temperature once sufficient neutron statistics has been obtained. The most common measurement sequences and on-the-fly analysis should be preprogrammed and easily accessible for the inexperienced user.
- 4. Archiving. Metadata associated with the experiment must be automatically archived and properly time-stamped so that the experiment can be "replayed" at a later point in time.
- 5. **Remote control.** It must be possible for users with the right authorisation, for example instrument responsibles, to monitor and control an experiment remotely, for example from laptops, smart phones, or tablets.

- 6. **Test runs and training.** It should be possible to make a virtual run of an experiment (a specified measurement sequence) prior to the real experiment.
- 7. **On-the-fly monitoring.** A user must be able to monitor the experiment and status of instrumentation on-the-fly during the experiment in order to enable the user to adjust or interrupt the experiment when required, rather than after the experiment is completed and it is too late.
- 8. **Fast operation.** Delays due to slow instrument control software should be avoided, thus, the user should feel that the reaction time is almost instantaneous.
- 9. **Support.** It should be possible to get support from experienced ESS personal whenever needed.
- 10. Advanced modes. For advanced and/or proficient users, including instrument scientists and local contacts, a Command Line Interface (CLI) and Application Programming Interface (API) are preferred rather than a GUI, because, for proficient users, it is faster to operate through a CLI and the API enables users to automate (also called sequence) experiments and for simply repeating a test run of the experiment for the real experiment. It should be mentioned that graphically based programming interfaces also can be made such as known from the control system NOMAD at ILL, which enable inexperienced users to do advanced programming (sequencing) of the experiment visually.

5.10.3 Guest scientist support and training.

There are three strategies for supporting inexperienced users:

- 1. Develop self-service systems for the guest scientists based on Graphical User Interfaces (GUI).
- 2. Supervise the guest scientists during the experiment by having an experienced local contact present during the experiment or alternatively, by letting the local contact control the experiment.
- 3. Train the guest scientists prior to the experiment by developing training sessions either virtually or through workshops.

The best strategy for a given instrument will be specific for that instrument and will most likely be a mixture of the three strategies. The benefit of a true self-service system is that it reduces the user support burden significantly. On the other hand, true self-service systems are expensive to develop and the Pareto principle is often quoted in this regard to state that it takes 80% of the time to develop the last 20% of the application. Thus, in many cases it might be cheaper to supervise the guest scientist on site or to educate them prior to the experiment. At existing facilities, guest scientists are often trained by the local contact during the experiment, but this option is presumably not a viable solution at ESS because data will be acquired at a much faster pace than at existing facilities.

5.11 Target control

Compared to the accelerator, for the target, there are about one order of magnitude less control signals. However, a major part of the activity of ESS will be concentrated in the target station, which calls for detailed consideration of its control system. The target is planning to use the same control system environment as both the accelerator and the instruments, based on EPICS, for the control of hardware. The level of integration between the accelerator, target and instruments is being defined.

For all these main systems, in correspondence to the various measurement devices, there will be control boxes, which will use the EPICS standard. All the information from the control boxes will be directed to a central control system. The control system must include also the interlock system, that is, the series of signals to stop the beam if something goes wrong.

The target control system is structured in the following way: on one side it includes basic input/output components, that is, those control measurements that concern the target system itself, not in relation with the rest of the facility. These are connected to industrial standard modules, basic PLC (programmable logic controller), delivered by suppliers. On the other side, there are control measurements related to the beam operation, which are very important for safety reasons. Control functions must be specified in order to process the signals from the various target measurements, in a useful way. Functions are shown in a display of controls. We consider briefly these different components

5.11.1 Basic I/O and component functions

The various control measurements related to the target are linked to industrial standard hardware systems. Examples of control measurements for the target systems are: leak detectors; temperature measurements; beam profile measurements; pressure sensors; wheel rotation measurements; flow measurements; synchronisation with the accelerator pulse timing; vacuum measurements and radiation monitors. It is important to define the list of signals coming from all systems within the target monolith and their related ancillaries to be managed by the control system. EPICS will be associated to the industrial hardware for the various controls. Different modes of operations will be needed, such as: stand by (target rotating but not irradiated), start up (progressive ramping up of the beam power) and beam-on operation.

The types of measurements can be divided into three categories:

- 1. Measurements of relevance for safety, where robustness and redundancy are critical
- 2. Measurements of relevance for operations, (that is, temperatures, flow rates)
- 3. Measurements to optimise performance, (that is, neutron flux)

Among the measurements of relevance for safety, there are measurements of radiation monitors, measurements of He leakage (we will have to specify the leak tightness), basic measurements of helium flow/pressure/temperature. Also, in the target station there are cryogenic systems, where it will be important to monitor the temperature; vacuum systems; water systems, where one can measure the temperature and its variation, hence the heat deposited. The most important safety alert to shut down the accelerator is when the wheel does not rotate with the prescribed speed or stops. Excursion of other parameters, such as temperatures of various components, pressures, flow rates, and as discussed below, also the beam profile are key shut-down interlock events.

Among the measurements on the target relevant to operation, there are: target deformation (measured with laser doppler vibrometers). Target temperature can be measured using thermocouples, which have been proven to be radiation resistant. The number and positioning of the thermocouples should be decided carefully in order to give indications of the temperature distribution. Additionally, continuous infrared imaging of the target envelope surfaces will be performed.

5.11.2 Beam operation

The target station control system will be interfaced with that of the accelerator. In particular, safety functions related with beam parameters will have to be defined. The footprint of the proton beam on the target will be optically monitored.

5.11.3 Target Protection System

The target protection system (TPS) will be implemented and maintained separately from the main control system, and will comply with safety regulations for nuclear facilities. It is not in the scope of the main control system to deal with nuclear safety classification. The majority of the systems for the target will not be safety critical. The current estimation is that about 80% of target control signals will be possible to control in the same

manner as signals of the main control system. The remaining 20% will be safety critical (under the jurisdiction of nuclear safety regulations) and will need to be controlled by means of the TPS. The main control system will be used to monitor the following:

- 1. Overall health and status of TPS
- 2. Readback of some of TPS signals in the main control system (but not the setting of these signals).

In general the TPS must make sure that the proton beam is instantly switched off in case of improper beam profile distribution on the target. Systems will have to be redundant, and possibly provided independently by the target and the accelerator. The beam profile monitors will be connected to the interlock systems. A series of events requiring protection functions are defined, such as: leaks of He coolant; signals from the accelerator (beam profile); and external events such as loss of power supply, fire, earthquake.

The TPS is currently not in the scope of work of the Integrated Control System department. The decision of who is responsible for TPS development has yet to be determined.

5.12 Online and offline accelerator beam modelling and simulation

Operators and accelerator physicists will decide which changes are needed to optimise the machine, for example to reduce losses and to steer the beam trajectory. They will be assisted by the online model: a virtual model of the accelerator that interacts with the User Interface as a real machine, and which allows parameter changes to be tested before applying them to the real accelerator. High level applications that will also use the online model to enable automatic routine tasks, such as loading the parameters from the running machine and finding the optimal configuration for a specific problem.

The implementation of the online model functionality will probably be based on the software HMI framework XAL, which is a Java programming infrastructure. XAL provides a hierarchal view of the accelerator and hides most of the underlying control system details. The hierarchy is database configured, facilitating application sharing across different beamlines, shielding the programmer from detailed knowledge of signal names. It allows wholesale updating of applications. The online model can be consulted for design values, for live machine values, or for user selected tuning values.

Offline simulations are necessary to understand the dynamics of protons and the possible instabilities generated by errors in the productions of the linac components, in the assembly or simply by random errors. The simulation codes will be flexible enough to include unexpected phenomena arising during the beam-commissioning phase. The codes will also provide single and multi particle capabilities in order to predict the widest range of situations that the operator can experience running the accelerator. The data required to construct the simulations, for example, systematic errors associated with component fabrication and alignment errors during installation, will be maintained in a database as a part of BLED.

Simulations and online models are not the same service: the online model must be fast and reliable for everyday operations in the control room. Simulations are the instrument to understand the issues of the dynamics. The online model will benefit from the experience of the simulations improving the capabilities of the control system. In the end this will be the basis for understanding and operating the machine with a control system that can learn and adapt to new situations by providing state of the art physics analysis to the accelerator physicists.

5.13 Organisation and management

In construction the ESS will accept in-kind contributions from project partners, instead of, or in addition to, cash contributions from member states. The Integrated Control System department will provide the organisation and infrastructure to make this kind of collaboration efficient for components within the ESS control system. A well defined set of procedures, interfaces and hardware that will standardise and integrate the deliveries of different collaborating partners will be provided. This will be achieved by using the Control Box on both technical (architecture) and organisational aspects of the control system. For maximum efficiency and cost management the controls should be integrated across all beam systems, including the injector, linac target, relevant conventional facilities and experimental stations. It is essential that some systems are shared, most notably, the timing system. All the interfaces should be defined as soon as possible.

6 Data Management

6.1 Data acquisition

At ESS, most data acquisition will be performed in event mode, as schematically shown in Figure 114, rather than in histogram mode. Event mode enables users to re-bin their data sets according to their specific needs. Thus, a time-stamped event is recorded every time that a neutron hits a detector with pixels in 1D or 2D. The time of the event is synchronised with the accelerator, so that every detected neutron can, in principle, be matched with the associated accelerator pulse. This synchronisation is performed through the timing system of the Integrated Control System.

In practice, a detector pixel has a dead time on the order of one microsecond after it has been hit by a neutron, in which a new event cannot be detected, resulting in a time resolution of the order of one microsecond for each pixel. A real-time data acquisition system resolution of 10-100 nanosecond enables the maximum possible time resolution to be obtained.

Event mode data acquisition can result in very high data rates – up to 300 M events or more per second from some instruments. The data acquisition control system is based on hardware rather than software, to ensure a sufficiently fast real-time system. At ILL a customisable CPU board from the Swiss company Creative Electronic Systems (CES) [118] is used for data acquisition. The use of the Integrated Control System will free valuable resources to be used to develop the ESS specific event-mode DAQ system, since it is anticipated that in addition to specific software, a number of custom hardware components may also need to be developed in order to cope with the extreme data rates. Moreover, EPICS [68] has support for some of the hardware used for data acquisition and can thus be used for the Control Box in Figure 114.



Figure 114: Schematic layout of the event mode DAQ system used at SNS, which may also be used at ESS.

6.1.1 User perspective

Two of the user requirements for the instrument control system relate to data acquisition. First, it will be possible to run an experiment in automatic mode, so that the experiment is modified automatically once a given criteria – for example, sufficient statistics – is obtained. Second, data reduction, visualisation and some analysis will be performed on-the-fly. There will be sufficient compute power available to perform data reduction and analysis, so that the results will be returned to the user as fast as possible after the raw data has been acquired. On-the-fly analysis will be performed onsite to reduce delay. Instrument control, data acquisition and analysis will be integrated.

6.2 Data storage

Data storage involves short time and long time secure storage, secure data transfer from production site to storage, methods to retrieve data remotely, and implementation of storage policies – for example, concerning the storage duration time, and public access to data. Many of the challenges related to these issues are currently being worked on in work packages in the CRISP [119] and PaNData [120] EU projects. The policies and frameworks developed in these work packages will be followed by ESS-DMSC, to the extent possible.

6.2.1 Technical requirements

Very high data acquisition rates as fast as 300 M events or more per second correspond to one PB per year for all instruments. Network data transfer will be designed to cope with these large data rates. The transfer of very large files and the computers for storage will cope with these rates and will be designed to store very large files (several GB). Fibres dedicated to ESS will ensure secure transfer from Lund to ESS-DMSC. Hard disks will be used for medium term storage, up to about one year. Tape stations will be used for long term storage. These tape stations will be able to store about one PB for each year of operation.

6.2.2 Backup and risk mitigation

An onsite cache storing capability (the Fileserver in Figure 114), which can store acquired data for up to 48 hours, will avoid data loss of data in the rare event of lost connection. Cache and data storage facilities will be mirrored to guard against breakdown or physical damage. At ISIS, for instance, the storage facility is mirrored twice. The mirror facilities will be placed in different locations, so that a fire (for example) will damage only one of the facilities. Data retrieval from multiple synchronised storage facilities will be optimised through load balancing for a better user experience.

6.2.3 User perspective

User requirements include:

- 1. Remote Access. Data will be accessible remotely for authorised users, for as long as they are stored.
- 2. Data Formats. Data will be easily accessible in a number of formats commonly used by the user community.
- 3. Public Access. Stored data will be available to the public after a certain period.

The last user requirement is being discussed in the community and is a way to maximise the outcome from the investments into large physics facilities. It could enable mining data from several different experiments by third party researchers, provided that sufficient information (meta data) is stored along with the raw data to make the experiment reproducible – another user requirement. The instrument control software is able to archive commands, parameters, and the physical state of the instrument and the sample environment – the so-called meta data.

The ICAT project [121] is a strong candidate for making a user interface for the data storage system that eventually will fulfil user requirements:

"ICAT is a database (with supporting software) that provides an interface to Large Facility experimental data and will provide a mechanism to link all aspects of the research chain from proposal through to publication."

ICAT is a collaboration between STFC, ILL, and the Diamond Light Source, and is being evaluated by ESRF.

6.3 Data analysis, visualisation and modelling

Data analysis, visualisation and modelling are essential for maximising the scientific outcome from experiments performed. Moreover, these tasks will be performed by the users (guest scientists).

Data analysis is performed in two stages. First, it will be possible to do a preliminary data analysis during the experiment to make sure that the experiment delivers the type of results which are expected, to ensure that the instrument performs correctly, and to guide the user in choosing the necessary and sufficient measurement times for each step of the measurement. The second stage takes place after the measurements have been completed and may involve modelling. Its goal is to produce as much scientific insight from the experiment as possible.

6.3.1 User perspective

User requirements include:

- 1. User-friendliness. User-friendly data analysis and visualisation software for all users of ESS independent of background, and different level of operations: simple (meaning preprogrammed common sequences of tasks) and advanced modes.
- 2. Look and feel. The same look and feel will be used for the data analysis software for all instruments. It is desirable for a user's familiarity with data analysis from other neutron or light sources to be transferrable to ESS, so that the look and feel of the user interface is the same across multiple facilities. A uniform look and feel for all ESS user-exposed software (instrument control and data analysis) will be an advantage both from a user perspective and also from a development point of view, reducing the development burden.
- 3. Automation. It will be possible to automate complicated analysis sequences. The most common analysis sequences will be pre-programmed and will be easily accessible to users.
- 4. Support. It will be possible to obtain support for data analysis before, during, and after the experiment.
- 5. Scientific computing. It will be possible for users to obtain assistance with interpretation of data through scientific computing.
- 6. Archiving. It will be possible for an authorised user to retrieve results from an analysis, anytime after the analysis was performed.
- 7. Training. It will be possible to obtain training in data analysis prior to an experiment.
- 8. **Compute power.** Users will be able to obtain the compute power needed for demanding data analysis tasks.
- It will be possible to perform on-the-fly data analysis.

6.3.2 Mantid

The user requirements associated with data analysis are similar to the user requirements associated with instrument control. They are not new. Software projects already exist that try to fulfil many of these requirements. The strongest contender is the Mantid project [122], initiated by ISIS and professionally managed by the TES-SELLA company [123]. Mantid was joined by SNS, which has allocated several developers to the project. ILL is considering joining the project as well. Mantid is based on open source software using a modern framework of C++ for computations, Qt for the GUI, and Python for scripting. Mantid is making use of best practice software development processes that are essential for maintenance and further development.

6.3.3 Remote access

The DMSC data analysis capabilities will be made available to users at their home institutions while the data resides at DMSC. In this way the powerful computers at DMSC and the high speed links to storage will make analysis efficient, and will avoid the unnecessary transfer of large amounts of measurement data.

6.3.4 Support and virtual experiments

Guest scientists with allocated beam time will be assisted by an ESS-DMSC employee from the time of acceptance of the associated proposal to publication. ESS-DMSC will develop training material (software and workshops) for prospective users of the data analysis software, and users will be able to practice operations and analysis associated with performing an experiment at ESS through virtual instruments. The user can virtually perform all steps associated with an experiment at ESS by passing "artificial data" produced by an instrument simulation program like McStas [124]. Instrument simulation software will be integrated with data analysis software. This will also be useful in the further development of Mantid and for analysing data for instruments based on Repetition Rate Multiplication.

6.3.5 Theory and scientific computing

Support with interpretation of data through scientific computing is high on the wish list in the user community, and is arguably a way to increase the likelihood of publishing, and to increase the impact of the published data. An expert group in molecular and materials modelling and simulation will be assembled with collective expertise in everything atomistic – that is, in biochemistry, chemistry, solid state physics, soft materials, chemical and material engineering – and will be equipped with required compute resources and software. The policy put in place for storage of experimental data at ESS will also be used for storage of data produced by this group.

A theory group might also be helpful before the actual experiment is performed to guide the experimental setup.

7 Conventional Facilities

7.1 Conceptual design (to start in 2012)

The new generation of ESS Research Laboratories will provide an attractive working atmosphere, including natural and intensive communication between the users and the permanent staff. This implies an excellent architecture, taking into consideration not only technical features, but also the aesthetics of the buildings, as well as an astute distribution of volumes. The on site life of users and staff will be rendered comfortable in welcome, housing, feeding, and in easy communication with close or remote scientific centres.

The ESS will be an important and spectacular part of European scientific potential. The image projected by the architectural design of the buildings will reflect this concept. Architecture will not be limited to buildings only. The 74 ha site will be landscaped to integrate it into perfect harmony with the environment. The architectural concept will also take into consideration the need for a modular, extensible design, so that architectural integrity can be maintained in the event of future extensions and additions.

Conceptual design work has two parts. The first part is to design a building program in which all requirements are identified for the plant, The second is an effort to study how to cost-effectively establish a structural design for the accelerator and target foundations. These studies will serve as input for the conceptual design of the facilities which will start when the conceptual design of the machine is ready.

- Site preparation
- Accelerator buildings
- Target building
- Instruments
- Office and laboratory buildings
- Auxiliary buildings

8 Safety

8.1 Licensing process

The licensing process of the ESS facility is given by three different legal acts in Sweden; the Radiation Protection Act, the Environmental Code and the Planning and Building Act. A formal notification was sent to the Swedish Radiation Safety Authority (SSM) in August 2010 saying that ESS intend to send an application for start of construction in the beginning of 2012 [125]. An important statement is that SSM regards ESS as a non-nuclear facility. However, due to the uniqueness of ESS as a spallation source SSM also state that special requirements (for example the same as for nuclear facilities) might be applied for ESS. After the notification, meetings between SSM and ESS are and have been held on a regular basis. Our primary goal is to produce a PSAR (Preliminary Safety Analysis Report) in which we describe the technical concept, potential risks and the mitigation of those risks, waste management and decommissioning of the facility. The PSAR will form the basis for the application of construction.

The Environmental Impact Assessment (EIA will be sent to the Environmental Court in the first quarter of 2012. Continuous work has been done for the facility planning layout process towards the Lund municipality in accordance with the Planning and Building Act. In these matters, ESS has a strong connection and cooperation with both Max-lab and the Lund municipality regarding the planning of the whole area northeast of Lund. An overview is given in Figure 115.



Figure 115: Overview of the licensing process.

8.2 General safety objectives

The European Spallation Source (ESS) is a complex facility where several hazards might occur. These hazards include radioactive hazards as well as non-radioactive hazards. Although ESS is not defined as a nuclear facility according to the Swedish regulation, ESS emphasises the objective of setting radiation shielding and safety as a main priority for all phases of the project from design, through construction and operation, to decommissioning.

When starting the operation of ESS, there will be no significant radioactive inventory. During operation, penetrating fast neutrons are generated in the target and by proton beam losses in the accelerator. The main inventory of nuclides will be in the target and thus it is in the target station where most radioactivity will be generated. Comparing ESS with other facilities, the radioactive inventory will be the same as for a about the same activity as a medium sized research reactor. Thus, the main hazards arise from radioactivity sources but other hazards, here named non-radiation hazards must be addressed as well. Examples are hazards originating from cryogenics, high-voltage, electromagnetic fields, heavy equipment, working on high heights, transports et cetera.

Concerning radiation, the ALARA principle (as low as reasonably achievable) shall be applied. This means that radiation doses have to remain as low as possible, or in other words that threshold doses may not be exceeded, if that can be reasonably avoided. On the other hand, ESS must have some dose limits for guidance. Otherwise, the design work would be impossible. Thus, in order to protect the ESS staff, the public and the environment, it is necessary that ESS states and defines specific General Safety Objectives (GSO). The GSO [126] will serve as a guiding document at ESS, giving necessary input of how to design the ESS facility.

8.2.1 Classification events

Table 46 lists the classification of events that will be used.

Classification	Event	Frequency [1/y]
H1	Normal operation	≥ 1
H2	Incidents	10^{-2} to 1
H3	Unexpected events	10^{-4} to 10^{-2}
H4	Design Basis Accidents (DBA)	10^{-6} to 10^{-4}
-	Beyond Design Basis Accidents (BDBA)	$\leq 10^{-6}$

Table 46: Definition of event classes for radiation hazard.

8.2.2 Radiation hazards and doses

The Swedish legislation differs between the doses permitted for people working in radiation environment (supervised) and the dose given to the public and environment. Therefore, the GSO is set differently for the staff and the public, as shown in Table 47.

Event	Description	Unit	Radiation workers	Non-exposed workers	Public (effective dose)
H1	Normal operation	[mSv/year]	10	0.05	0.05
H2	Incidents	[mSv/event]	20	0.5	0.5
H3	Unexpected events	[mSv/event]	50	5	5
H4	Design Basis Accident	[mSv/event]	100	50	50

Table 47: Summary of GSO limits regarding doses.

8.3 Defence-in-depth

The ESS is designed with the "defence-in-depth" principle [127]. The International Nuclear Safety Advisory Group (INSAG), part of IAEA, defines five levels of defence in depth for future nuclear facilities:

- 1. Prevention of abnormal operation and failures.
- 2. Control of abnormal operation and detection of failures.
- 3. Control of accidents within the design basis.
- 4. Control of severe plant conditions, including prevention of accident progression and mitigation of the consequences of severe accidents.
- 5. Mitigation of radiological consequences of significant releases of radioactive materials.

An outcome of 1 and 4 is that the ESS facility shall be designed with Safety Barriers (SB). These are physical barriers constructed in order to contain the radioactive inventory of the ESS facility in case of different events. The barriers will not be equal with regard to strength but the will be used in order to mitigate a possible event/incident/accident at different parts of the facility. Table 48 lists the different barriers for the different parts of ESS.

Section	SB number	Safety barrier
Target	1	Target envelope
	2	Confinement/crypt vessel
	3	Target building
Accelerator	1	Linac tunnel entrance
	2	Accelerator shielding
Neutron beamlines	1	beamline guides
	2	beamline shielding
Instrument buildings	1	Instrument shielding
	2	Instrument building
Waste disposal building	1	Container/vessel/package
	2	Building

Table 48: Safety barriers (SB) for different components of the ESS facility.

8.4 Radiation shielding

Possible exposure of radiation to ESS workers and the public is the criterion for design of the shielding. Shielding will be necessary for the target inventory, the accelerator tunnel and at the instruments. The shielding of the target and the accelerator tunnel will be permanent and designed according with the general safety objectives of ESS. Working procedures and area classifications are additional components to further limit radiation exposure. Engineered features as fences and occupancy factors, operational limitations and indirect sources like the air activation are accounted in calculating doses. Layout of the shielding design will be drawn to engineering standards and provisions will be made for accounting in uncertainties in, for example calculations and drawings. A safety factor of 3 will be used for the shielding estimates. Other important protective feature of the shielding is to ensure design requirements for equipment. The shielding design will be done to accommodate to potential upgrades of the accelerator. Thus, the monolith shielding and other non-replaceable systems at the target station will be installed to handle 7.5 MW, whereas replaceable systems and shielding will be installed to handle 5 MW.

Prompt radiation. MCNPX, FLUKA and PHITS computer codes are intended to be used for the estimation of the prompt mixed particle fluxes and further ambient dose rates H * (10) by folding these fluxes with the corresponding flux to dose conversion factors.

Residual radiation. For residual radiation estimates the computer codes to be used are using different strategy. FLUKA code is estimating the residual field (activation and contact gamma dose rates) on-line with the prompt radiation run. It means that all information including irradiation history should be supplied once in the beginning. For MCNPX or PHITS, adjacent computer codes needs to be coupled with them, namely CINDER90 and DCHAIN-SP-2001. Different techniques are used and compare in order to validate the reliability of the estimations. Usually simple handbook calculations with adjustments and assumptions for the specific case are used to be compared with the results of the very complex and rigorous Monte Carlo analysis in order to build credibility in both sets of results.



Figure 116: Monolith cross section (SNS-STS, 2008).

8.4.1 Target shielding

Target monolith. An important feature of the target station is the elimination of the primary shutters within the shielding monolith. This makes the monolith shielding simpler and more effective. The target station includes individual secondary beamline shutters near the monolith, to minimise the residual dose during maintenance and repair operations on nearby beamline components. Beyond the shutters outside the iron-shielding boundary are located choppers. Both shutters and choppers will be handled vertically for maintenance and replacement. The proposed arrangement of the shielding monolith is similar to that shown in Figure 116.

For the shielding of the target assembly a combination of proper shielding materials (as cast iron, heavy concrete, et cetera) is supposed to be used and therefore optimised. The guess size of shielding monolith is based on calculations completed for existing similar facilities by scaling to 5 MW. For SNS second target the shielding monolith was sized at 7.5 m at 3 MW power. Preliminary estimates of the bulk shielding dimensions obtained by scaling the ISIS design are shown in Table 49. The parameter for optimisation of the basement shielding thickness will be driven by the activation of the earth underneath. Additionally, in order to reduce the risk of the migration of the contaminants arising from the earth activation below the target a geo-membrane is intended to be used.

Angle to proton beam [degrees]	Total [m]	Iron [m]	Heavy concrete [m]
25	7.5	5.5	2.0
55	6.6	5.0	1.6
75	6.0	4.5	1.5
105	5.4	4.0	1.4
135	4.5	3.4	1.1
165	4.0	3.0	1.0

Table 49: Minimum thickness required to comply with a constraint limit of 2.5 μ Sv/h.

Shutters. The design of the shutters aims to stop any residual radiation at shutdown of the beam. Minimising the shielded handling flask of the shutter is another goal. The shutter should limited the residual gamma dose coming from the cave at 8-10 m from moderator to less than 10 μ Sv/h. Proposals for materials to be used for the optimisation of the shutter core (zone that close the opening of the neutron beam) are: Pb, Fe, and Cu. Preliminary value of the thickness of the shutter core is driven by the gamma spectra residual after shut-down.

Neutron guide shielding. Curved neutron guides project horizontally from the core vessel penetrate the shielding monolith. The neutron guides are installed inside the beam tubes starting at 2 m distance from the view face of the moderator. Neutron beamline shielding beyond the target monolith boundary will depend of the specific set-up of the experiment. In order to simplify access to the beamlines a shielded bunker extended for several metres is consider in the concept. Detailed optimisation of such shielded bunker is required in the optimisation phase of the project.

Hot cells. The design of the hot cells is based on the existing previous experience. The shielding consists of successive layers of stainless steel and concrete having several windows. Provision will be made for temporary storage of at least two spent targets.

Potential hazard in case of accident. During the selection process of Target material a hazard index was calculated weighting the inventory nuclide vector with release fractions and effective dose commitment factors per inhalation. The accident release fractions used are roughly representative for a worst-case type of accident involving loss of integrity of the target material and are usually used for screening facility radionuclide hazard [128]. The assigned release fractions are basically based on the physical chemical characteristics of the individual elements. A particular attention was done to W that was assigned as a semi volatile since the available information from the fusion energy shows that W dust produced via disruption can be released into airborne during an accident. The inhalation dose coefficients used for this analysis originating from the International Commission on Radiological Protection and from the IAEA [129, 130]. Two different target concepts were studied. The solid W target and the liquid LBE concept. A mercury target at 5 MW was considered as reference. The results show clearly that W target concept has the lowest accident release potential. Strong evidence in the favour of the W concept was found also in reference [131] as finding of the analysis of the toxicity of the target concepts analysed here. Considering radionuclide inventories weighted by physical/chemical proprieties

it resulted from the comparison that W target hazard index is slightly lower than for the first approach while the ratio of LBE target hazard index remains almost unchanged.

8.4.2 Accelerator shielding

ESS does not foresee any construction problem regarding the shielding for the accelerator. The challenge is to fulfil the environmental requirements related to radiation and at the same time optimise the construction of the shielding in a cost-effective way. One of the contributors for the accelerator regarding the amount of radiation reaching the public is the specific pathway of activated soil being transported via the groundwater. This will occur as one contribution during normal operation. According to the GSO the total allowed dose rate to the public arising from the accelerator during normal operation is a maximum value of 0.03 mSv/y as design criteria. Including the pathway through the groundwater.

Another example is the expected event "Beam loss" which could result in a 5 MW beam pointing up through the ground, reaching a person on the surface. The GSO states that the received dose rate from this specific category of events is not allowed to exceed 0.05 mSv. Together with a safety system, cutting off the beam, this event will define the need of radiation shielding between the accelerator and people on the surface, which is a different criteria and thus give rise to another shielding thickness and other possible solutions compared to the groundwater issue. ESS has discussed several possible alternatives for the shielding of the accelerator tunnel. Further discussions are needed as well as updated calculations. The final optimisation is a balance between cost of material (soil, steel and concrete), water level of groundwater and shielding requirement.

9 Integration

Integration involves a wide range of technical systems and personnel, all working together. The various tasks for the integration team cover a wide range, from fitting two parts in the machine together, to preparing for the installation of components with tight alignment tolerances. The main task is to gather data from all interests, to review them, and to support the organisation in finally getting a technical solution that is possible to build, assemble and align according to requirements. The integration team will plan the survey and alignment together with cable tray routing during the pre-construction phase. More precise integration strategies will be presented later, in the Technical Design Report.

9.1 Survey and alignment

A range of conventional technical systems are being integrated together to ensure a smooth design, planning, construction, installation and commissioning process. Active pre-alignment is one of the key points of the project. Components must be pre-aligned with respect to a straight line over a length of approximately 500 m. The highest priority in the global strategy for survey and alignment is to have unified and correct 3D models, drawings and data. This is necessary to get a good final result during installation.

9.1.1 Determining component positions

The alignment strategy has three steps:

- 1. Integrate and merge drawings and data.
- 2. Set up the Sitewide Coordination System with a survey network.
- 3. Fiducialise.

Integrating and merging drawings and data. A number of inputs from various areas are needed to get the correct alignment of the machine. Each area of inputs is essential for the end result. ESS is working on the processes and procedures from the pre-construction phase through to the operations phase, in order to establish a solution for maintaining alignment. It is essential to keep track of the alignment in order to maintain a high performance spallation source. A close relationship between survey and alignment, design, physics and construction is absolutely essential. Any changes to any part of the machine will be documented so that all responsible parties are aware of the change. This methodology will result in tremendous savings to the project. It is important that these groups work as a team, in order to build a quality project on time, within budget, and safely.

Design input. The mechanical design consists of a large number of components and systems. The design includes all equipment and components for the machine and instruments, and also for the installation fixtures and stands. The different solutions with regards to function and installation are being standardised.

Physics input. All ideal positions (coordinates) of each component on the beamline and through the target station out to the instruments are generated by physics simulations and calculations. This data is the foundation for the machine performance. The data are transformed so that the survey and alignment team can merge the data into a unified solution.

Construction input. Constructing a facility where a high tech machine will be installed requires a different approach from a normal construction project. One of the foremost requirements is that the construction uses a Sitewide Coordinate System and survey network, in which a number of secondary survey monuments are tightly integrated into the buildings.

Integration and merging. The Complete Plant Layout (CPL) is the 3D overall model that consists of all coordinate locations, all buildings, all mechanical parts including fiducials, all survey monuments and the idealised beamlines throughout the accelerator and to the instruments. All conduit locations for piping, transfer lines and electrical locations are included in the CPL. The integration team and the survey and alignment team are preparing and setting up the 3D overall model, and establishing the procedures that will be used to maintain the correct inputs from, and outputs to, all interests.

The Sitewide Coordinate System and the survey network.

Sitewide Coordinate System. The unified coordinate system that is needed during construction and operation is provided by the Sitewide Coordinate System (SCS) shown in Figure 117. The SCS will be used in metrology by installation and alignment groups, and by other users. The system is Cartesian, with three axes (E, N, and Z) that are straight lines oriented at 90 degrees to each other. The SCS axes do not follow the curvature of the earth. The origin of the SCS is at a reasonable distance off the ESS site, so that all values of E and N coordinates are guaranteed to be positive, on site. The origin is theoretical – it is not a physical survey monument.



Figure 117: The Cartesian Sitewide Coordinate System. The origin is off the ESS site, so that all on site values of E and N coordinates are guaranteed to be positive.

ESS survey network. The survey network consists of different types of primary monuments and penetrations into a grid of a secondary monuments. The final network has a line of sight view of components to be installed, with monument locations that depend on the final layout of the plant. Global survey network planning is far enough advanced to be a viable asset to the project in the present and in the future. An example of a sitewide network, at the SNS, is shown in Figure 118.

Primary monuments. A small number of primary survey monuments will be installed, and their exact locations will be determined (and maintained) in the SCS. They will be very stable and immobile, allowing the movement of the secondary reference points to be monitored and recorded in the fixed SCS frame. Figure 119 (left) shows an example from SNS. Primary monuments locations will be determined, and the monuments will be installed, when the building design is sufficiently finalised. Changing a building height after monument installation could render a monument useless, if lines of sight to other primary monuments are lost. The network of primary survey monuments will be presented more precisely in the TDR.


Figure 118: Primary and secondary monuments in the SNS "Precision Network".



Figure 119: Examples of SNS survey monuments. Left: A primary monument. Centre and right: Floor and wall mounted secondary survey monuments.

Secondary Survey Monuments. Secondary survey monuments, such as those shown in Figure 119, will be installed and maintained inside all buildings and tunnels where accurate surveying and alignment activities need to be performed. The required number and their placement will be finalised before building construction begins. Secondary monuments may move, for example as buildings settle. These movements will be recorded and the coordinates of monument locations will be adjusted against the primary survey monuments. In some cases penetration points will be necessary to get a clear line of sight between primary and secondary monuments. Technical solutions for floor and wall monuments are being determined.

Fiducialisation. A component pre-alignment feasibility study is being performed. This requires knowledge of:

- 1. A stable and known alignment reference.
- 2. The capacity and accuracy of sensors.
- 3. Compatibility with software systems.

9.1.2 Proton and neutron beamline coordinates

The idealised proton and neutron beamlines are (approximately) radial to the centre of the core monolith in the target station. The SCS locations of these lines – plus the vertical offset of the moderator focal points – set the basic structure for describing the component layout for each beamline, for use by the survey and alignment team, and others. Work processes, measurement equipment and techniques are being established to connect the idealised beamline component locations with other required data and drawings.

Cost of measurements. A careful effort is being made to accurately identify the necessary alignment tolerances. Setting the tolerances too tightly increases costs in both the equipment and also in installation. Each component is being evaluated. Where a looser tolerance is acceptable, effort is being made to reduce costs. Physics, engineering, design, et cetera, will call out realistic alignment tolerances that are required, and not more.

Survey and alignment instrumentation. Several instruments for alignment will be used. An investigation is taking place to identify necessary equipment and software. Equipment examples include optical transits, optical level, industrial theodolites, total stations, laser-trackers and 3D laser scanners.

9.2 Cable trays

A number of systems are cross functional across the entire plant. Information and requirements for these areas are being established, to get good, well defined technical solutions. One such system is electrical cabling. A well controlled system is being provided in order to systematise and keep control of the different types of cables, and their individual identities. The cable tray strategy presented here will be described in more detail in the TDR.

Strategy. The cost and time used during the engineering and drafting design phases are substantially less for cable tray wiring systems, than for conduit wiring systems, for projects like the ESS that are incompletely defined before design start. Final drawings are completed and sent out for bid or construction more quickly for a cable tray wiring system, than for a conduit wiring system. Cable tray simplifies the wiring system design process and reduces the number of details. Cable tray wiring systems are well suited for computer aided design drawings. A spread sheet based wiring management program will be used to control the cable fills in the cable tray. Dedicated cable tray installation zones alert other engineering disciplines to avoid designs that will produce equipment and material installation conflicts in these areas. A cable can easily enter and exit a cable tray anywhere along its route, allowing for some unique opportunities that provide highly flexible designs.

9.2.1 Space allocation

Space allocation methods are being developed for planning all cable routing, for both process systems and for electrical cabling. Figure 120 presents a typical cross-sectional view of the accelerator tunnel, along with tentative space allocations.



Figure 120: Space allocations in a typical accelerator tunnel cross-section.

9.2.2 Standardisation

A number of activities are taking place in order to establish a standardised solution for all cable trays. Information that is needed to determine the number, size and routing of cable trays is being assembled – for example; system, cable function, cable description, cable diameter and bend radius, number of cables including spares, need to separate from other cables, start point and end point, et cetera. A decision on what types of cable trays will be used in what environment is also in process. A variety of technical solutions can be adopted in different environments, depending on safety, fire et cetera. Appropriate installation standards are also being investigated, including which cables should placed in cable trays. This includes conventional facility cabling, controls cabling, and machine and instrument cabling.

10 Energy Systems

Responsible, Renewable, Recyclable and Reliable: A Conceptual Design of Energy Systems for ESS.

10.1 Design goals and parameters

Guiding principles. The site decision for ESS was made on the basis of a submission from the Scandinavian host countries that included a firm commitment to build a "sustainable" research centre (ESS Scandinavia 2008). This was based on an energy strategy called Responsible, Renewable and Recyclable, meaning that the future ESS would be energy efficient, run on renewable energy sources, and recycle waste heat. In recognition of the paramount importance of availability for the success of the facility, and that the sustainability of the facility would be first and foremost decided by the success of the research conducted, a fourth key word was added: Reliable.

The conceptual design of the ESS achieves the goals set up for Responsible, Renewable, Recyclable and Reliable. Furthermore, implementation of the Energy Strategy in the design will deliver savings and revenue in the operation phase, compared to a conventional facility design, which may amount to as much as 15 million euros annually. Similarly, the savings in carbon dioxide emissions compared to a conventional solution amount to 165,000 tonnes per year. Operational costs in general fall outside the scope of this report, but are discussed in this section in as much as cost optimisation either acts as a guiding principle for the design or results from the efforts to reduce climate impact.

10.1.1 Local conditions

High-voltage power. Regional high-voltage power lines are adjacent to the site. These are two-way, providing the possibility of redundant supply lines, as specified in the ESS 2002 design (ESS 2002). The short circuit power in the lines is specified in Table 50, divided into power during normal operation and the minimal level "n-1 level" in the event of faults. The need for short circuit power is not settled presently, the significant parameter depends on the ESS choice of modulators. A realistic reference value is specified in Table 50. If necessary, by means of relatively simple rebuilding, the regional grid can be strengthened to accommodate ESS needs so that the short circuit power in case of faults can be increased. The cost of the necessary changes is estimated at 1-2 MSEK and will be weighed against other alternatives on site.

Scenario	Capacity [MVA]
Present network situation	
Normal operation	≈ 2600
n-1 operation	≈ 850
New network topology	
Normal operation	≈ 3600
n-1 operation	≈ 1900
New network topology plus a	
new 130 kV cable connection	
Normal operation	≈ 4450
n-1 operation	≈ 3275

Table 50: Short circuit power on the 130 kV level, at the new ESS substation.

Residual voltage	Duration [s]				
	0.01 to 0.02	0.02 to 0.1	0.1 to 0.5	> 0.5	
85% to $95%$	1	1	0	0	
70% to $85%$	0	2	1	0	
40% to $70%$	0	1	1	0	
$<\!40\%$	0	0	0	0	

Table 51: Number of voltage dips between July 2011 and November 2011, registered at Sege.

The occurrence of voltage dips from half a cycle to a few seconds cannot be eliminated completely. Transient over-voltages do occur in the sub-transmission electricity network. Transient over-voltages propagate to distribution networks, and can damage equipment in network-user facilities. Complete power outages are rare, but do occur, perhaps once or twice a decade. Table 51 shows the number of voltage dips during the period from July 2011 to November 2011.

Magnetic fields. In face of a possible alternate line routing in the regional grid in connection with establishment of ESS and MAX IV, a calculation regarding magnetic field contribution from the 130 kV line and the branching of this line toward Lund Eastern Substation has been performed, for four alternative line designs. The preliminary site of establishment for ESS may, according to the calculations, during normal operational conditions in the 130 kV grid be exposed to a maximal magnetic field contribution from the lines by about 0.1 μ T. During situations of fault condition in the grid, the contribution may amount to maximum about 10 μ T. The duration of such fault conditions is estimated to be maximum one second per occasion. Such fault conditions are estimated to occur at ten to one hundred times per year.

District heating. The City of Lund has a district heating system that includes the nearby City of Eslöv and as well as the Town of Lomma and thus supplies around 800 GWh of heat per year, albeit with significant seasonal variation. The operating temperature of the system is a minimum of 75 C. Plans exist to connect this system with the systems to Landskrona and Helsingborg. This would lead to a total available heating demand sufficient to make use of all ESS heat even in summer. Also, a geothermal system has been in use in Lund for decades, to supply the base heating load. This system could be converted to and aquifer to store heat seasonally. This itself would also have the capacity to absorb the heat from ESS.

10.1.2 Energy inventory

In order to be able to design appropriate energy systems and to focus attention on energy efficiency, an energy inventory is conducted and maintained continually, with increasing level of detail. This inventory is not just a static list. It is the basis for an energy flow map. It also includes not only energies, but also temperatures, because preserving temperature levels was identified to be a key issue for the value of recycled heat. The Energy Inventory was first based on the 2002 ESS design (ESS 2002), with adaptions for the Lund site and design, but has since been continually updated to match specifications from the on-going design update in the ESS facility when possible. In other cases, the inventory data is based on observations from other laboratories, primarily Spallation Neutron Source at Oak Ridge, Tennessee. The operating times used in Energy Inventory calculations are specified in Table 52.

Mode	Duration per year [h]		
Full operation	5200		
Down-time	1900		
Intermediate (eg start-up)	1700		

Table 52: Operating hours per year used in Energy Inventory Calculations.

10.2 Cooling systems

General design philosophy. The power demand of ESS in normal full operation is specified in Table 53. Almost all of this energy will need to be cooled off through controlled cooling systems. Only a minor amount will be lost to the surroundings through losses or exhaust air from ventilation systems. Therefore, the cooling demand through water based and temperature-controlled system is also close to the total power demand. One of the ESS key words is recyclable. Therefore the cooling system should be designed so that a large part of the energy can be recovered. In order to lower recovery costs and enable waste heat recovery, it is of considerable value to keep temperatures as high as possible, both for possible revenue from heat sales and savings in electricity demand. There will therefore be three different temperature levels for cooling.

Section	Power demand [MW]
Ion source, including initial linac section	3
RF Power Source	17
Helium cryogenic system for the linac	4
Helium cryogenic system for the target	3
Target station	2
Instruments	1
Cooling system and others	8
TOTAL POWER DEMAND	38

Table 53: Power demand in different sections.

Cooling demand. Information regarding cooling demands and acceptable temperature levels in various types of equipment are summarised in Table 54. Cooling demand data in MW refer to full-scale operation. During ramping-up, standby and downtime the cooling demands are smaller.

Section	Waste heat production	20 C	40 C	90 C
	[GWh/yr]	[MW]	[MW]	[MW]
Ion source & warm linac	7	0.7	0.1	0.4
Klystron gallery & cold linac	68	3.0	1.9	6.9
Helium system (linac)	30	0.0	1.5	2.5
Helium system (target)	16	0.0	1.0	2.0
Target station	25	2.0	0.0	2.5
Instruments	5	1.0	0.0	0.0
Miscellaneous	23	2.5	0.3	1.6
TOTAL	174	9.2	4.8	15.9

Table 54: Cooling demands and temperature levels.

Centralised cooling and heat pump unit. Three temperature levels, chilled, medium and high will supply the cooling system. Input and return temperatures for these loops, and the temperature change ΔT , are specified in Table 55. The lower levels will be needed if conventional cooling systems for comfort are used. However, there are alternative technologies available, and preferred. If the conventional systems can be avoided the higher temperatures could be applicable. Heat Pumps (HP) will be required for chilled water loops, as well as for the intermediate temperature loops. The highest temperature loop will have separate return temperatures for different types of equipment. The mean return temperature is high enough to just use ordinary plate heat exchangers to transfer the heat to the district-heating network. The number of heat pumps and heat exchangers for the different loops are specified in Table 55. The heat pumps will lift the temperature of the energy cooled off to a temperature level high enough to allow use in the district-heating network.

The cooling system will include a back-up system, ready for use in case of a breakdown in the normal system. The back-up system could be based on spare machines similar to those normally used. There may be opportunity to use some of the low-temperature waste heat in the area surrounding the ESS. For this purpose, we plan for at least one heat exchanger that will supply heat externally at temperatures below the district

heating temperature level. In case of major downtime periods, heat supply from the district heating to the ESS might be required. For this purpose, one additional heat exchanger will be installed in the heat pump building.

		Chilled water loop	Medium temp loop	High temp loop
Input temperature	[C]	10 - 20	30 - 40	50 - 80
Return temperature	[C]	17 - 25	40 - 50	60 - 90
Temperature difference, ΔT	[C]	5	10	10
Number of heat pumps		3	2	0
Electric power per pump	[kW]	3	2	n.a.
Number of heat exchangers		9	4	2
Electric power per exchanger	[kW]	10	10	10

Table 55: Cooling loop performance and required equipment.

10.2.1 Cooling distribution systems

A basic overview of the distribution systems is found in Figure 121. For cooling purposes, the high and medium temperature systems are connected only to the process equipment in the linac and the helium plants. The low temperature system needs to be connected to all the ESS buildings. For heating purposes, there is a need for a widely distributed heating network. Preferably, the heating demands could be supplied from the high or intermediate temperature level cooling systems. Thereby the number of distributions systems could be decreased and possibly the heat pump power demand lower. Much of the cooling will be done in secondary systems. The water in these systems will be purified to a de-ionised level. Other liquids may be preferable in specific sub-systems. There will be a large number of such systems, shown as red-coloured squares in the figure. The number of connection points between the primary distribution systems and the secondary systems are not known at present.

Example: Cooling the klystron gallery. Some of the equipment in the klystron gallery requires secondary cooling systems with de-ionised water due to the risk of radiation contamination. For control purposes the secondary cooling systems in klystron gallery will be divided into several sections, each connected to a cooling sub-station. This requires five cooling substations, each supplying secondary cooling water at the three temperature levels to be used in the klystron gallery. In order to enable a constant high temperature cooling, a variable flow is necessary. A schematic figure of one klystron and its modulator is shown on the right of Figure 96.

Each of the cooling substations will be equipped with:

- Three heat exchangers, one for each temperature level, transferring heat between primary and secondary cooling circuits
- Distribution pumps with full redundancy for each secondary cooling system
- Water treatment equipment for supply of de-ionised water into the secondary systems

There are at least five cooling points in this set-up:

- The modulator will be cooled mainly with the intermediate system. The oil in the modulator and the klystron require cooling at the same temperature and will be connected to the same cooling circuit.
- The klystron body requires medium cooling temperatures.
- The collector will be cooled at a high temperature.
- The circulator could be connected to the collector cooling system.
- The dummy load will be cooled at a high temperature. Cooling of the dummy load varies considerably between different modes of operation. Therefore each load is equipped with a separate cooling water tank, and heat is transferred to the cooling system through a local heat exchanger.



Figure 121: Distribution piping schematic. This does not represent the actual piping location.

10.3 Reliable electrical system

Design specification. The design of the electrical supply and distribution system, as shown in Figure 122, is aimed to ensure that electrical supply is not a limiting factor for the availability of the facility. This means insuring an adequate security of supply, including redundant systems and reserve power system, as appropriate. It also includes adequate uninterruptible back-up power to enable the orderly powering down of the facility and supply sufficient emergency power. Unwanted fluctuations in the grid voltage are one of the main reasons for power supply trips, which leads to unscheduled beam interruptions. The electrical system must supply sufficient quality correction to ensure uninterrupted operation, including powered equipment to compensate for voltage dips. Aside from electrical issues, other identified demands include vibrations, magnetic fields and systems for reduction of risk of fire or explosions.

There are also defined demands for how ESS may affect the surrounding grid. ESS is responsible for ensuring that unallowable electrical disturbance, as accentuate harmonics and flicker, do not appear in the local network. The processes in the ESS that have an effect on the power quality must be identified and their disturbance must be controlled. How much accentuate harmonics and flicker the 130 kV network can receive without disturb the public network depends on the dimension of the short circuit power.



Figure 122: Line diagram of the electrical distribution systems, including substations and power backup.

Receiving station. The switchyard area for the receiving station is about 100 m by 200 m and will be placed as closely as possible to the 130 kV region line for as short a 130 kV cable connection as possible to the station. It may be appropriate to incorporate redundancy of supply into the design, as suggested. In order to have redundant supply to ESS the 130 kV line could be split in two parts and these two lines connected separately to the receiving station. The conceptual design includes redundant supply, meaning connection to two separate incoming power lines and two main transformers. The cost of this redundant supply will be weighed against reserve power alternatives and the added security of supply that the alternatives provide. The switchyard area design is indoor, with air-insulated 130 kV switchgear with transformers and medium voltage switchgear. Should centralised reserve power units be required, these could also be located here.

Substations and Site Power Distribution. A number of substations will be located in the plant. A standardised similar network substation will be developed for the easy and safe operation and less spare parts. The internal medium voltage grid can be constructed with loops or radial feeds. A loop solution has been chosen for the conceptual design for added flexibility.

Redundancy and back-up power. As it is unlikely that sufficient security of supply can be achieved by other means, reserve power units will need to be deployed. There are large variety of technologies to store electricity energy for continuous quality power, including capacitors, flywheels, batteries, backup generators and combinations of these. With the rapid development of battery technology, reliance on mechanical or combustion-based power may be possible to eliminate, for almost all power outage scenarios. If combustion reserve power is necessary, there are two options for its location in the plant, either centrally positioned reserve power units or individual distributed reserve power units. The annual number of unplanned outages is shown in Table 56.

	2007	2008	2009	2010	2011
Mörarp-Sege	2	2	1	1	0
Karsefors K-Knäred	2	0	2	1	2
Åhus V-Tomelilla	5	1	1	4	1

Table 56: History of the annual number of unplanned outages on 3 local 130 kV overhead lines.

Corrective Equipment. Voltage interference such as harmonic distortions, frequency variations and transients from the Modulators RF signals will mostly be eliminated with filters and galvanically separated transformers. Appropriate protection from transient overvoltage will be added. For the most sensitive systems, such as the helium compressors and the klystron modulators, a filter integrated with smart circuitry and a battery and/or capacitor is the preferred option to supply voltage correction and first-order back-up power.

Direct current option. As an alternative for handling voltage quality issues, and for improved performance and availability, an option will be explored to convert the low-voltage bus bar before the klystron modulators to direct current. This would also significantly simplify the modulator design.

10.4 Renewable energy and other energy issues

The Renewable target entails that ESS is to be supplied via 100 % renewable energy sources. The background for this target is that ESS wishes to avoid the increase in CO2-emissions that would otherwise be caused by the electricity consumption in the plant. ESS is achieving this by ensuring that the equivalent amount of new renewable electricity generation is built. The chosen renewable plants should also contribute to secure stability in cost of electricity over time for ESS, and thus avoiding the risk of a reduction in research capacity due to future increased energy costs. ESS should aim for a mix of different renewable energy sources, as a variety in energy sources gives stability in price and security of supply. The location of the electricity generation plants should be in European countries that are participating in the ESS project, with a preference for locations as near the ESS facility as possible. The chosen renewable energy sources should be in line with the sources that EU has approved as renewable energy, today a list from application of grant from NER300.

Building heating and cooling systems. Comfort heating and cooling for the various buildings on site are a small part of the ESS energy profile, but the numbers are not negligible. The medium temperature cooling water will be used for internal heat demand, meaning that all heating needs will be covered without cost and carbon emissions. In fact use of medium temperature heat internally will reduce electricity demand in the cooling system. Reduction of heating demand is therefore not a priority, but cooling demand must be minimised. For the cooling that cannot be avoided, cooling systems driven by heat, such as sorptive cooling, are preferable. Seasonally, "free cooling", meaning use of outdoor ambient temperatures may be the best option. For lighting, a low voltage system and LEDs are preferred.

Energy management. Studies at SNS show that insufficient energy data is detrimental to operations [132]. Integrated control systems are have been demonstrated to pay operational dividends [133]. An extensive system of measurement and data collection, connected to integrated systems for control and maintenance can improve availability and reduce operational costs.

Data management centre. Cooling for the data management centre in Copenhagen is not included in the design described above, due to differences in local conditions that have not yet been fully explored. A district heating system is available as a heat recipient, but the tax conditions may be significantly different. A cooling system based on heat pumps and recycling is the preferred option.

11 Conclusions

This Conceptual Design Report is the result of the intense and increasing effort over the past 12 months which is but one step – albeit a very important one – on the road to the construction of the European Spallation Source after 20 years of planning. It is a milestone, and like all milestones it does not indicate having arrived, but rather it is a significant step on the journey. The document therefore should be read in that context. As you read its 250 pages, the project design and planning has already moved on. Currently there are around 250 people from the almost 50 contributing partner labs working on the project compared to 100 at the beginning of 2011. Many of these people have been part-time. In 2012 this effort will double and the CDR will be superseded by the TDR – the Technical Design Report – at the end of the year. At that time much other documentation will be available, including an updated cost report, which will allow partner countries to take a well-informed decision to proceed to the construction of the ESS in 2013 so as to achieve our main goal: the delivery of neutrons before this decade is out.

A Commissioning and Operations

Commissioning is planned in three major parts:

- 1. Infrastructure and conventional facilities
- 2. Accelerator and target
- 3. Instruments

A.1 Accelerator commissioning

The installation of accelerator and target components will begin as soon as occupational readiness is achieved after buildings and the installation of infrastructure like electricity, water, ventilation and communications are completed. The different subsystems will be installed and taken into operation in steps separated by readiness reviews, ensuring that all dependencies of one subsystem on another are fulfilled and verified. Accelerator readiness reviews will allow beam commissioning to begin. Detailed commissioning plans will be written for all systems during the construction phase, at the same time that all necessary procedures, software tools and instruments are developed. Commissioning goals will define what performance to achieve before commissioning turns into operations.

The rate at which accelerator equipment can be installed will to a large extent depend on the delivery schedule for critical components. ESS will saturate the worldwide production capacity for components such as klystrons, modulators and cryomodules. For instance, it is expected that the more than 200 klystrons currently foreseen can be manufactured and delivered at a rate of at most one per week. Even if the number of klystrons can be reduced or if the delivery rate can be increased somewhat, it is clear that components will arrive over a substantial period of time – several years – that is a significant fraction of the total time from now until neutron production starts, and which is similar to the time it will take to complete the infrastructure and the conventional facilities.



Figure 123: The three commissioning stages with the lengths of the different linac sections, including the HEBT up to the first dipole magnet that bends the beam towards the surface, drawn approximately to scale in the horizontal dimension.

Staged commissioning. The commissioning plan is based on the concept of a stepwise completion of the infrastructure and conventional facilities. In order to use the available time in an efficient manner, the linac tunnel, the klystron building and the infrastructure are built in three stages, including supporting infrastructure such as electrical power, cooling water, piping for cryogenic fluids, et cetera. Each stage allows the complete installation of a section of the accelerator and its associated equipment. Section commissioning will take place while work on the buildings for the next stage continues to take place. The three stages illustrated in Figure 123, comprise:

- 1. Normal conducting linac, that is, ion source, LEBT, RFQ, MEBT and DTL.
- 2. First part of the superconducting linac with spoke resonators, all medium beta elliptical cavities and some high beta elliptical cavities
- 3. Second part of the superconducting linac, including all remaining high beta elliptical cavities and HEBT

Stage 1 requires that electrical power, cooling water and other services are installed. Cryogens are not used until stages 2 and 3. Cryogenic plant commissioning for the accelerator is thus part of stage 2.

Portable beam dump. Ionising radiation created by the beam will limit the extent to which beam commissioning in the early sections of the linac can occur while construction work continues downstream. A portable beam dump will be moved along the linac tunnel as installation work proceeds. This beam dump dissipates the energy of the accelerated beam and acts as a radiation shield between the beam and the construction work taking place downstream. The portable dump will consist of carbon blocks, possibly water cooled, that are surrounded by concrete blocks acting as a radiation shield or wall. It will be able to dissipate in the order of 1 kW. The portable dump receives beam at the nominal energy (at that position in the accelerator) and at the nominal current, but the beam pulses will be much shorter than nominal, down to $10 - 20 \mu$ s, and the pulse repetition rate will be much lower, so that radiation can be kept at acceptable levels. It will still be possible to verify full operation of a majority of subsystems during each of the three commissioning stages, however, because the instantaneous beam power reaches its nominal value. Full power beam commissioning will be performed when the spallation target is in operation, since the accelerator itself will not be equipped with a beam dump that can handle the full average power of 5 MW.

Acceptance testing before installation. "Commissioning" here refers to the testing and start up of the linac and its associated equipment after final installation in Lund. Hardware components will arrive from factories and laboratories around the world for installation. All major components will be tested before they are sent to Lund. This includes ion source, RFQ, DTL tanks, cryomodules, RF sources and many other items. Klystrons, modulators and other commercially manufactured equipment will be tested at the manufacturer. Linac structures will be tested at dedicated facilities at several collaborating accelerator laboratories. The normal conducting accelerator up through the RFQ will be tested for an extended amount of time, in the order of 6 months, at full power and with beam before it is delivered to Lund.

Stage 1 – **Normal conducting Linac.** The first commissioning stage encompasses the normal conducting part of the linear accelerator. It thus includes the ion source, low energy beam transport, radio frequency quadrupole, medium energy beam transport and drift tube linac. This section is altogether around 30 m long. It is being discussed whether this part of the linac building will be a tunnel with a similar cross section as the rest of the tunnel, or if it will be an underground hall of bigger dimensions. In the latter case, there can be a test area for ion sources, and possibly also for developments and for tests of an upgraded front end with beam if this would be required in the future. It is estimated that the assembly and installation of well prepared and tested accelerator components will take 3 - 6 months after occupational readiness of the building is achieved. This includes RF installation, which takes place in parallel with linac installation. Beam commissioning then lasts 1 - 3 months. Both installation and beam commissioning are performed according to detailed plans worked out during the construction phase. Detailed plans and reviews are also made for beam instrumentation, software tools and the environment in the control room needed to steer, visualise and model the behaviour of the beam. Protons are brought from one diagnostic device to the next during beam commissioning, while properties such as position, size, emittance and stability are measured and compared to calculations. Safety interlocks and protection systems are tested in parallel, with continuous radiation monitoring.

Stage 2 – **Superconducting linac.** The linac has three types of superconducting cavities: spoke resonators, medium beta elliptical cavities and high beta elliptical cavities. Production of these will largely take place in parallel. The production of high beta cavities and cryomodules, in particular, will start early because of the large number required. All the spoke cryomodules, all the medium beta cryomodules, and a significant fraction of the high beta cryomodules will be commissioned in the second commissioning stage. The accelerator cryoplant will also be commissioned in stage 2. There is considerably more installation work to be performed in preparation for stage 2, compared to stage 1, because of the large number of cryomodules and power sources and because of the need for cryogenics. Nonetheless, it is likely that the time required for superconducting installation is set by the rate at which cryomodules, klystrons and modulators can be manufactured and delivered, rather than by the amount of work necessary on site. The commissioning procedure is basically similar to stage 1, except for the additional steps involving the cryoplant and cold mass cool down.

Stage 3 – **High beta elliptical and HEBT sections.** The final part of the linac tunnel houses the high beta elliptical cavity cryomodules and the high energy beam transport to the target. The linac tunnel joins the target station building in the vicinity of the first dipole in the HEBT dogleg that takes the beam up to the level of the target. The target building also houses the final horizontal section that delivers beam to the target, and a permanent tune up beam dump in an extension of the linac tunnel, behind the first dipole. The target and

the target building are likely to become available after the linac tunnel and the associated klystron building are finished. It is therefore likely that the portable beam dump will be used during beam commissioning at the beginning of stage 3, with short pulse lengths and with a small duty cycle. The requirements on building and services are the same as for stage 2, and the time needed for installation of the acceleration modules and the RF sources are again likely to be determined by their delivery rates. The commissioning procedure is also the same as in stage 2.

The HEBT section inside the target building also needs to be commissioned at low power, in order not to activate the area by neutrons back streaming from the target, and ensuring that access is readily made if problems are found during the initial target commissioning. This commissioning must wait, however, until the target installation is complete, since there is no room to install the portable beam dump after the tune up dump. Full power commissioning will begin when the target is ready, testing all aspects of linac operation that cannot be reached at lower powers. This includes effects of beam loss, beam loss monitoring and related safety interlocks, and issues related to total heat dissipation in normal conducting cavities, cryostats, power couplers, klystrons, modulators and other equipment.

A.2 Target station commissioning

The time frame for accelerator commissioning will be rather long, as explained in the previous section. The target station will be the last major machine component to be commissioned. Target commissioning will demonstrate both the appropriate performance and also the safe functioning of the target systems, during operation (with beam on target) and also during maintenance. The commissioning includes the neutron production systems (target, moderators and premoderators, proton beam window, et cetera), the ancillary systems and the safety systems (shielding, confinement, et cetera).

The first stage of target commissioning will be performed without any beam on the target, allowing for the correction and adjustment of parameters as necessary. This stage will proceed in parallel with accelerator commissioning, up until beam commissioning on the tune up beam dump system. Some safety functions will be tested in this stage (usage of portable sealed sources, et cetera), without creating any active inventory. The second (and most important) stage starts when the proton beam is first delivered to the target. Procedures for the second stage commissioning are still being defined. They will include the following activities:

- Ramping up the proton beam power. Irradiation will start with very low power on target (on the order of one percent of the nominal 5 MW). Some low power measurements will be performed before progressively increasing the power, with intermediate stabilised plateaus.
- Investigating the performances and safety of the target station, to match the expected operating and licensing requirements.

Target beam commissioning thus includes the following tests and qualifications:

Accelerator to target interface. Beam profile measurements will be performed by both accelerator and target. The correct functioning of the beam profile monitors is essential as the peak current density will be controlled at all times during irradiation.

Target station monitoring. Validate and understand control signals from the target, such as pressure sensors and target temperature measurements. When possible, physical parameters will be measured directly by independent redundant systems through the target control system, in order to cross check and validate the normal output signals.

Target station to instruments interfaces. Signals from instruments. First neutrons will be detected by the instruments.

Radiation protection. Radiation measurements. Radiation monitoring at some key points of the facility will be performed, including dose measurements at the beam exits and radiation gas monitors.

Confinement function. Internal confinement function – safety barriers for radioactive contamination, and zoning for helium and hydrogen hazards. These functions are assured by the HVAC and confinement devices (penetrations).

Handling systems. Handling systems will be tested before active beam commissioning.

Target ancillary systems performance. Very low power target commissioning may be performed without some ancillary systems, but all ancillary systems will be fully operational well before full power operation.

Target control system. The interdependences of different target control sub-systems will be tested, such as transients and protective actions (threshold, automatic shutdown, et cetera).

B Comparative Target System Concept

A baseline target was chosen for ESS offering the best balance between neutronic performance, safety and development effort. The objective of studying a comparative solution is to present a broader picture with possible alternatives in the licensing process and to accumulate knowledge for an eventual re-evaluation of the situation in the case the baseline option meets unexpected difficulties, be they technical, due to cost or development time. The choice of a Lead Bismuth Eutectic (LBE) target as a comparative solution is drawn from experience with:

- liquid metal targets (mercury) at major pulsed spallation neutron sources SNS (commissioned in 2006) and JSNS (commissioned in 2008).
- the MEGAPIE neutron production target that operated for six months at SINQ-PSI.

Liquid metal targets have undergone all stages of design, commissioning and operation (and ongoing postirradiation analysis in the case of MEGAPIE) over the last decade or so, for the very specific application of neutron production at MW power levels. In this sense they are the best understood targets, with clearly identified advantages and disadvantages. This is especially important in regard to the ancillary systems, which are complex but where experience is available. It would be possible to adapt existing monolith designs and layouts from SNS and JSNS to ESS, with relatively minor changes. For example, the MEGAPIE target was designed with stringent geometrical constraints, in order to fit into an existing facility originally developed for a solid target, integrating liquid metal pumps and a heat exchanger within a tight cylindrical envelope undoubtedly more challenging than ESS.

The LBE target design builds on previous experience, adapting the flow pattern around the target to enable a two-stage approach to its implementation:

- 1. A target with a window suitable for the lower beam power to be expected during commissioning of the facility, and capable of full power operation albeit with a relatively short lifetime.
- 2. A windowless target with an increased lifetime, capable of accommodating potential power upgrades beyond 5 MW.

B.1 Practical and technical motivations for LBE

History of use of lead and LBE. 80 reactor-years of operational experience in Russian submarines with LBE-cooled fast reactors. In 2006 MEGAPIE at PSI became the first MW-class liquid metal target.

A lead-based target is licensable in Lund. The MEGAPIE licensing experience is applicable to ESS. A mercury target is more challenging to license than LBE, due to high volatility and disposal issues.

MEGAPIE collaborative experience. ESS could benefit extensively from the MEGAPIE experience in which specialists in Europe, the U.S. and Japan designed custom target systems following a quality assurance (QA ISO 9001) system for operating a safe target.

Lead/LBE is planned in future projects, such as reactor core coolants for fast reactors and targets for accelerator driven systems (for example, the MYRRHA project).

Material databases on lead and LBE. The OECD/NEA Handbook on LBE and lead properties [134] is a comprehensive source of available data on LBE and lead, for applications in a radiation environment.

Well known layout, handling and maintenance schemes. Existing schemes (ESS2003, SNS, JSNS) can be directly implemented or improved, rather than developing new schemes for a rotating target.

Advantages over mercury. There is a greater margin before boiling point is reached. The boiling point at 1 atmosphere is 2216 C for LBE, and 357 C for mercury. Retention factors can be applied to lead for many of the radioactive species in an accidental release scenario. LBE is solid at room temperature, simplifying the disposal process.

B.2 LBE target system

The approach to the design of the LBE target is modular with window/windowless target, pump, heat exchanger, pool and containment modules. Since the windowless and window target modules are almost identical geometrically and thermo-hydraulically, all other modules are independent of the chosen target module. The overall layout is shown in Figure 124. The target and both moderators are installed on separate trolleys, which allow for their horizontal extraction from the proton interaction region into a hot cell in order to perform maintenance. The first safety barrier, monolith and hot cell arrangement are similar to the SNS and JSNS layouts. The major difference with SNS and JSNS is having moderators on a trolley. This requirement is driven by the target geometry, as described below.



Figure 124: Layout of the comparative LBE target design, showing separate target and moderator trolleys, and coupling to the monolith via inflatable seals. Extraction of both moderators and the target is performed horizontally, into a hot cell that is not shown.

B.2.1 Target module

Target with a window. The module sketched in Figure 125 consists of a proton beam guide with a safety window, an inflow channel leading to a nozzle producing a uniform block velocity profile, a U-bend and an outflow duct. The flow is pumped upwards, then directed into an inclined channel (± 2 degree angle) and accelerated by a nozzle into a channel that is inclined at an angle of 15 degrees relative to the horizontal plane. This leads to an extremely stable block velocity profile that does not suffer from instabilities. The proton beam enters the liquid metal through a solid wall that is approximately 2 mm thick, and which is nearly parallel to the bottom wall of the inflow channel The depth of the channel is chosen for optimal moderator positioning.

There is no sudden change of flow direction in the proton beam interaction zone, in contrast to other target designs like MEGAPIE, SNS, and the METAL:LIC design in EURISOL. Stagnation points that typically result in cavitation and vibrations are thereby omitted. The proposed U-bend gently turns the fluid flow. A small inclination angle enables the flow component perpendicular to the beam to transport the fluid across the beam in a short time. The counterflow quickly removes the hot LBE from the beam interaction zone. This is an advantage for pulsed beams, as successive beam pulses interact with fluid that was not previously subjected to the beam.

The target module is installed above the LBE level in the pool, so that the target module completely drains when the pumps are not operating. An emergency beam dump behind the interaction zone with temperature monitors is wired to the machine protection system, to handle short term transients in which the LBE may not provide sufficient beam stopping power. The target module operates when the LBE level reaches the top of the inflow channel. This is easily monitored. The pressure inside the target module at the highest elevation is slightly above the vapour pressure of LBE. Inside the target module the pressure is given by gravitational



Figure 125: Sketch of target and moderator modules showing on the left the proton beam guide and in red, the proton path through the beam guide and into the LBE.

pressure and small losses. This implies that the pressure at any location within the target module is below ambient pressure. The target module is attached to the pool by a plug to allow replacing the target module structure (excluding LBE inventory).

Windowless target. This target module differs mainly by the removal of the window, establishing a free surface flow with a shape that closely follows the (removed) window. The geometric dimensions of the windowless target module are identical to those of the window target module. The window limits the lifetime of the structure, and removing it substantially prolongs the target module lifetime. The window also limits the beam power, because it reaches the maximum temperature of the structure. The windowless option therefore provides a large margin for proton beam power upgrades.

The proton beam is directed onto a free surface, so that no solid structures are subjected to the proton beam. The proton beam is guided through a vacuum environment before hitting the target. Thus, the free surface separates vacuum and the liquid metal target material. In general targets are enclosed in a safety shroud to safely enclose the activated inventory in case of an accident, limiting unwanted migration of activated material. In the windowless target the free surface is a natural boundary between the LBE and vacuum. The role of the safety shroud is necessarily more pronounced, since this natural boundary cannot be counted as a safety barrier.

A double walled beam guide welded to the target module and a double walled beam entrance window (BEW) act as safety barriers. The BEW is placed downstream of a proton beam window (PBW), between the PBW and the free surface. A cover gas in the gap between the double walls is monitored for leak detection. Potential splashes from the free surface are collected in the beam guide and returned to the pool. Vapour is condensed by cooling distinct sections of the beam guide, ensuring that the beam entrance window is protected from direct contact with LBE. This permits the use of low cross-section aluminium alloys.

LBE cavitation and vaporisation is expected during the proton beam interaction, and some recovery time is necessary. The 15 degree tilt angle results in a cross velocity that is one quarter of the axial velocity. An axial velocity of about 1.6 m/s is sufficient to ensure that no fluid is overheated, from being subjected to multiple beam pulses. A shockwave is generated due to thermal expansion following each pulse. Shockwave dispersion is enhanced by obstacles installed in the flow channel, and perhaps by entraining a small amount of cover gas into the liquid metal. Free surface flow instabilities must also be controlled, since upstream travelling surface waves could potentially disrupt the surface. The speed of gravity waves is about 0.3 m/s, well below the anticipated flow velocity, so that the free surface flow is supercritical with respect to surface waves. A hydraulic jump forms when the supercritical flow enters the pool and becomes subcritical.

B.2.2 Pump and heat exchanger modules

The target requires a high flow rate, low pressure, and a head pump. Possible options are impeller pumps and electromagnetic pumps. An electromagnetic pump is preferred if moving parts need to be excluded. An axial impeller pump is proposed, delivering high reliability and the possibility to install the motor in the cover gas inside the target enclosure. The impeller is submerged in the pool. The impeller housing is part of the pump module that is pushed into the heat exchanger module on the low pressure side. The vertical motor axis transfers angular momentum to the impeller through a set of gears. Liquid metal lubrication bearings constrain the axis.

The heat exchanger handles the 3 MW of proton beam power that is deposited in the target, with some margin. Heat transfer on the liquid metal side is very efficient due to the very high thermal conductivity. Spray cooling is foreseen on the secondary side, due to the high heat transfer flux rate. Water spray cooling can achieve heat transfer rates of 1 MW/m^2 , or oil can be used as in the MEGAPIE target. Another possibility for improving the heat exchanger is to change the secondary cooling fluid to another liquid metal. The helical pin heat exchangers employed in MEGAPIE can be installed in ESS, by increasing the number of cooling pins to reach higher powers.

B.2.3 Pool

The pool is designed for a long lifetime, potentially up to the lifetime of the facility. The pool is dimensioned to accommodate potential future upgrades of the target without the necessity to replace the activated LBE. LBE expands during solidification so that freezing requires special care. Potentially unacceptable stresses are avoided by electrically heating the pool, keeping the LBE permanently molten once the target becomes operational. The LBE inventory is the major mass of the whole target. It is also the major activated mass of the target. The pool vessel is equipped with a number of remotely operable fixtures to which modules can be attached. These fixtures can tolerate material swelling due to irradiation.

B.2.4 Cover gas system and containment

The cover gas system (CGS) handles the volatile radioactive and non-radioactive inventory of spallation products released from the LBE in the target. In METAL:LIC a CGS similar to the MEGAPIE system [135, 136] is integrated into the pool module. The potential for a target fire can be excluded if a liquid metal is chosen as primary coolant for the heat exchanger. In addition it is possible to install a gas absorber in the pool. In that case, the CGS would act as a system for gas sampling and for handling unexpectedly produced gases.

The modular target is installed in a double-wall containment. The gap between the walls is filled with cover gas that is monitored for contamination. The containment walls are thin, preferably made from materials with low absorption cross sections, low activation potentials, and sufficiently low gas production. The containment is at ambient pressure and is therefore not subjected to high mechanical stresses. Low activation materials permit the containment to be opened for maintenance with reasonable effort. Contamination of the containment by condensates like lead is suppressed by installing non-heated sections near any free surfaces to act as cold traps, and by guiding vapour flow. The cold traps stay operational during the maintenance or replacement of modules, so that migration of activated materials is minimised when the containment is opened. The proton beam enters the containment through a double safety window built from suitable magnesium aluminium alloys, and cooled (probably) by water. Evaporation cooling can realise high heat transfer rates. A window breakage is identified by detecting tracers, inside or outside the containment, that have been added to the coolant.

B.3 Thermo-hydraulic analysis

The commercial code Star-CCM+ [137] and standard LBE properties [134] are used for thermo-hydraulic analysis, after proton beam energy deposition calculations using MCNPX. Transient simulations at nominal flow rate yield the time-resolved thermal results in the LBE and surrounding structure shown in Figures 126 and 127. These temperature ranges do not have any impact on the corrosion resistance and the resistance to liquid metal embrittlement of the T91 steel, given an oxidising condition of the liquid metal [138, 139]. Furthermore the maximum velocity does not exceed 2 m/s, and so erosion of the natural oxide layer can also be excluded [139].



Figure 126: Mean temperature distribution for the window target module.



Figure 127: Transient maximum temperature for the structural material for a proton beam repetition rate of 20 Hz.

The free surface in the windowless option is simulated using the volume-of-fluid technique, with LBE vapour at 1 Pa as the light fluid. Free surface instabilities are weak – they are analytically estimated to not exceed 1 mm. The transient simulations that generated the snapshot shown in Figure 128 demonstrate that surface waves flow downstream, so that disturbances produced by the beam interaction disappear before the next proton pulse arrives. Simulations using the smoothed particle hydrodynamics with typical tensile stress data for liquid metals address cavitation, pressure wave propagation and the potential for splashing at the free surface. These simulations show that splashing fluid cannot hit the beam entrance window, a results that is to be verified experimentally at KIT.



Figure 128: Development of the free surface flow (iso-surface of volume-of-fluid = 0.5).

B.4 Materials and lifetime

The MEGAPIE project has provided data on structural materials for LBE targets, generated through dedicated research programmes during its conception, notably the Spallation Target Irradiation Programme at the SINQ facility at PSI. Furthermore, the MEGAPIE target itself is currently undergoing an extensive post-irradiation analysis, which will provide valuable data especially on structures directly exposed to the incoming proton beam and in contact with flowing LBE. The materials of interest are the ferritic-martensitic steel T91 for the segment of the target directly exposed to protons in the window-target module, SS316L(-N) for the other structures of the target module, and perhaps AlMg₃ for the containment, as at MEGAPIE. Corrosion data is extensively available [134], complemented by ongoing studies mostly within the MYRRHA project.

Component lifetime is a crucial factor in determining the feasibility of the LBE target, especially since it will drive the availability of the facility. The latest Monte Carlo simulations of radiation damage, including two moderators and reflectors in the geometry description, show 47 dpa/y in the window, 14 dpa/y in the side wall, and 15 dpa/y in the bottom wall, assuming 5,000 hours per year in operation. The current acceptable limit for T91 under proton irradiation is 10 dpa, which would lead to 5 target changes per year. However, it is not clear that the window portion receiving the proton beam has a critical structural role. Rather, its function is to separate the LBE from the proton beam vacuum. Further, a conservatively small gaussian profile was assumed for the proton beam, with $\sigma_V = 15$ mm and $\sigma_H = 50$ mm. It is relatively straightforward to adopt a parabolic or even flat profile that would lead to half the dpa/y values quoted above.

B.5 Activity and accident scenarios

Spallation reactions will produce large amounts of isotopes, both stable and radioactive. All isotopes can alter the physical and chemical properties of the target material and structural components. In addition, radioactive isotopes will contribute to the total activity of the target, which must be quantified in order to plan for maintenance and disposal of target station components. The releases of relevant isotopes are defined under general safety cases during normal operation and under various accidental scenarios. Preliminary extrapolations from MEGAPIE indicate that the radiological impact is manageable for an LBE target. The accidental release of gaseous and volatile elements into the cover gas system (closed system) and their release into the environment (open system) will be investigated further.

The inventory of radioactive isotopes used in the MEGAPIE licensing procedures was calculated for an irradiation of 200 days with a proton current of 1.4 mA at 575 MeV. The activity of the noble gases and hydrogen was limited to a build-up over 50 days, the period for venting the expansion volume to a decay tank. The amount of volatile nuclear reaction products in the LBE at the end of irradiation was calculated to be 64.1 g, of which 43.6 g is radioactive. This is expected to be about one order of magnitude less than an LBE-based ESS target at the end of its irradiation. The ESS numbers are higher because of longer irradiation times, higher power, higher operating temperatures, and larger gas volumes. Theoretical and experimental studies demonstrate that polonium evaporation to the cover gas in an LBE-based target at typical operating temperatures (300 C) is low. For open systems the evaporation rate remains small for temperatures below 600 C. Mathematical expressions relating evaporation rate as a function of temperature and polonium concentrations can be used in evaluating polonium release in accidental scenarios. They were successfully applied in the MEGAPIE licensing procedure.

Large differences between MEGAPIE and ESS are predicted for the activities of volatiles in the cover gas phase, ranging from only slightly higher values for thallium, lead and bismuth up to a factor of about 105 for caesium. In ESS these nuclides are produced with a factor of 5 higher intensity and have a roughly 50 times larger accumulation time in a 1000 times larger gas phase volume. Furthermore, their equilibrium gas phase concentrations increase with temperature. The temperatures used for predictions were 250 C for MEGAPIE and 300 C for ESS. However, the dilution of the volatiles in the liquid metal is 10 times higher in ESS. The gas phase activity in the cover gas of ESS is predicted to be 1000 times higher than MEGAPIE for the most hazardous elements, mercury and polonium.

Various models were used to estimate the release of activity from LBE spilled at MEGAPIE, including parameters such as total pool surface, cooling and solidification rates, and interaction with water. These showed that 13.5% of the material could be released from the target facility, namely 2.2×10^8 Bq, 3.2×10^2 Bq, 4.2×10^{12} Bq, 8.6×10^{11} Bq and 4.2×10^{11} Bq from mercury, polonium, krypton, xenon and tritium respectively. The amounts of polonium predicted to be released for the MEGAPIE licensing were calculated before more recent and more reliable data became available, and were overestimated by a factor of 3. Activity released from a thin film of LBE adhering to the walls of the target was also estimated and turned out to be the dominant term in an accident scenario. The study assumed a film thickness of 20 μ m, corresponding to a mass of 3.5 kg (0.4% of total LBE in the target) deposited on an area of 16.7 m². Cooling curves of different target components were extracted to estimate the release of mercury and polonium in three different scenarios. The highest activities were found to be 9.8×10^{11} Bq and 6.0×10^8 Bq for mercury and polonium, respectively. Several additional issues had to be addressed for MEGAPIE licensing, to prove that the population living in the environment of the facility would not be exposed to doses higher than 1 mSv even under severe accident scenarios.

ESS benefits greatly from MEGAPIE experience, in addressing safety issues during the design phase. The main conclusions are:

- 1. Mercury is by far the largest contributor to the cover gas activity, due to high volatility and lack of chemical retention in LBE.
- 2. The total radioactivity in the cover gas is roughly three orders of magnitude larger at ESS than in MEGAPIE, due to the larger cover gas volume.
- 3. ESS will have a larger total inventory of volatiles, but also a larger volume leading to similar concentrations, vapour pressures and release rates.
- 4. The horizontal layout of the ESS target has many advantages over the vertical layout of MEGAPIE in accident scenarios, leading to much smaller potential spills of activated LBE into the monolith.

B.6 Handling and maintenance procedures

Moderator maintenance.

- 1. Open moderator inflatable seal.
- 2. Remove moderator from monolith by moving moderator trolley including moderator shielding.
- 3. Optional: separate moderator shielding from moderator plug using a small mounting trolley. Reinstall shielding plug and close monolith using temporary seal.
- 4. Move moderator into moderator cask for further maintenance in moderator maintenance area.

Target maintenance.

- 1. Shut down pump module, drain LBE into pool.
- 2. Remove moderators.
- 3. Open beam entrance window plug, replace beam entrance window by maintenance plug, store window in window cask.
- 4. Open target inflatable seal.
- 5. Remove target from monolith by moving target trolley including target plug shielding.
- 6. Optional: separate target shielding from target plug using a small mounting trolley. Reinstall shielding plug and close monolith using temporary seal.
- 7. Move target trolley into target hot cell.

Target module replacement (1-2 weeks in total).

- 1. Remove target.
- 2. Pressurise target module to ambient pressure from cover gas storage volume.
- 3. Open outer pool lid.
- 4. Open target module plug.
- 5. Move target module into disposal cask.
- 6. Insulate target pool with temporary target module plug, or install new target module.
- 7. Depressurise from cover gas storage volume.

Heat exchanger and pump module replacement (2-4 weeks in total).

- 1. Remove target.
- 2. Pressurise target module to ambient pressure from cover gas storage volume.
- 3. Open outer pool lid.
- 4. Open target module plug.
- 5. Move target module into disposal cask or storage cask.
- 6. Open inner pool lid.
- 7. Lift heat exchanger and pump modules vertically. Allow remaining LBE to drain and freeze.
- 8. Move modules into disposal cask.
- 9. Install new modules.
- 10. Optional: mitigate radioactivity by closing pool with temporary lid, and performing remote handling inside closed insulated environment.

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