ESS Instrumentation Task: Update and Workplan
November 2001 –May 2002

Dear Colleagues,

We trust that you have had great summer holidays and a busy conference season. It was nice to meet many of you at in September at ICNS2001 in Munich, Germany, and the 7th ESS General Meeting in Seggau, Austria. After the decision on the target stations following the Engelberg ESS SAC meeting, based on the science case and the great input from you with our study of generic instrument performances, the ESS project gained in strength and focus. Other key decisions have also been accomplished by now, which opened up the way for ESS to go ahead full speed towards the next main milestone of the project. This is to formally present the ESS proposal complete in all necessary details to the European science community and scientific authorities in 16 May 2002, with the scope to achieve a positive decision on funding by the end of 2003. The proposed ESS will be a stand-alone facility with a total of 10 MW beam power, primarily dedicated for neutron scattering research in science and technology. It will be open for other, supplementary applications, such as fundamental physics, nuclear physics, muon research, irradiation work, etc. The ESS reference accelerator concept already provides a fully satisfactory approach to build on. Potential advantages of using superconducting cavities in the linac will be vigorously explored and the accelerator design will be comprehensively reviewed in due course in order to take full advantage of all technical enhancement opportunities to emerge. The target/moderator design is in the process to enter the complex phase of "engineering realities" in which the neutronic performance will be established and optimised for target station layouts reflecting all engineering details of the real facility as it will be built.

ESS Day One Reference Instrument Suite

The next milestone for the Instrumentation Task is to establish, study and evaluate a reference suite of about 20 "day one" instruments for ESS, distributed between the two target stations. This accomplishment will serve a number of crucial purposes:

1) It will be part of the ESS proposal to be presented in May 2002, in order to give a specific idea of the huge research capabilities ESS will offer.

2) It will underpin the scientific case for ESS, to be presented by the Scientific Advisory Council (SAC) in May 2002.

3) It will serve as science driven benchmark to allow the ESS project to define and optimise the configuration of both target stations, including the number and choice of moderators and neutron beam extraction optics, and also for fine-tuning of accelerator parameters.

4) It will provide basic input for the ESS conventional facility design in terms of space requirements, general layout, shielding needs, utilities etc.

5) It will help the Instrumentation Task Group to identify and address key R&D needs for the realisation of an outstanding instrument suite for ESS, which will decisively surpass any other facility existing now or by the time of ESS coming on line..

A first version of the “ESS Day One Reference Instrument Suite” is attached as an appendix. It is essentially the one recommended by the ESS SAC meeting at ILL, 5-6 November 2001, with a few question marks filled in. ESS SAC members stressed that “threshold” instruments and applications should be given particular priority, in view of things that cannot be done with the flux of the existing sources, even with best possible instruments, but will become feasible at ESS. Innovation was also stressed as an important priority, together with nevertheless including a number of workhorse instruments with very high throughput.

The choice of the target station (50 Hz short pulse or 16.7 Hz long pulse) is obvious for most instruments on the list, but there are some cases where the choice depends on the specification to be defined. One example is the use of shortest pulses for best resolution. Using choppers 10-20 μs FWHM, sharp pulses can be achieved on the long pulse source in the full wavelength band (eventually using wavelength frame multiplication). For cold/cool neutrons this is much shorter than the poisoned short pulses, and offering in addition the capability of adjusting the pulse length according to the experimental needs between the shortest and some 200-300 μs. This can open up the way to achieve considerably higher resolutions than possible today (except for hot neutrons). This new opportunity can be of interest for and extend the capabilities of some of the machines on the list, e.g. engineering diffractometer.

Moderator Options

For the choice of moderators, recent “physical model” studies by the ESS target-moderator task (i.e. without full engineering details) confirmed that there is little to gain by a number less usual, alternative target configurations (such as flux trap geometry, alternative reflector materials,…). Therefore for the next phase of our work in the Instrumentation Task we will need to continue to use the 31-12-2000 analytic reference moderator performance models we have used by now. It will only need to be updated when ESS calculations on “engineering target/moderator models” become available. We should, however, identify potentials for making use of more innovative moderator design options already at this stage. The followings have been proposed by now:

a) *Methane or similar moderator*: If it becomes technically feasible at all, it could provide up to 2 – 2.5 times higher peak flux in short pulses in the 1.5 – 3 Å range for de-coupled and de-coupled poisoned moderators. The final gain factors might be considerably less, depending on engineering details not yet known. No substantial gains compared with coupled H_2 moderators are expected. To establish feasibility will need several years of R&D and it cannot be assumed in the next phase of our work. Nevertheless, it is important to identify the instruments which would take advantage of such a moderator, in order to keep the options free for an eventual modification of the reference design in few years time by replacing one the now planned moderator.

b) A *composite moderator* has been considered by SNS and it was found inadequate for short pulses (because of poor lineshape). It consists of a thin H_2 moderator layer in front of a H_2O moderator, giving a spectrum which is between that of the two moderators (roughly a 50 % - 50 % weight combination). It should be reconsidered for coupled moderators, primarily on the LP target station. It can be of interest if a broad wavelength band combining that of the thermal and cold neutron ranges is of prime interest to the expense of flux in both ranges (cf. 50-50 weight combination). Such a moderator is certainly feasible, it needs to be studied though.

c) *Be reflected cold moderator*. It is a proposal by E. Pitcher et al at LANSCE. It is expected to provide 50 % flux increase for $\lambda > 4$ Å, but a much reduced flux at shorter wavelengths. It is certainly feasible, but needs to be studied. It might be a candidate, as the composite moderator, for one of several cold moderator faces viewed on the LP target station, for applications such us very low q SANS.

d) Horizontally *extended size moderator for hot neutrons*. The reference moderator size, 12 cm x 12 cm is sufficient if (supermirror) guide neutron beam extraction is used, however it provides a rather small solid angle for direct view by a sample at typically 10 m or further away. In the ESS horizontal injection, wing moderator geometry it is impossible to extend the moderator size vertically, but it could be doubled horizontally without much loss in brightness. This would offer some 2 fold flux increase at $\lambda < 1 – 1.2$ Å wavelengths at the expense of horizontal beam divergence. (The eventually unfavourable impact of the latter could be eliminated by a vertical scattering plane design, such as MARI at ISIS). Such an enhanced flux moderator is certainly feasible, and it is being studied.

e) A final point on moderators is that all cold (H_2) moderators, including the coupled one, will provide equal length or shorter pulses in the < 2 Å wavelength range on the SP pulse target station than de-coupled or poisoned ambient water moderators. Thus a coupled cold moderator might be an advantageous alternative to poisoned moderators for high-resolution thermal and hot neutron work

f) The feasibility of an enhanced integrated flux, low-resolution hot neutron moderator (proposed to be achieved by the direct view of the reflector) is also being studied, e.g. short wavelength for single crystal work.

It is of particular importance to assess all reasonable target station and moderator options for the instruments. Several possible choices for each instrument might have to be considered, in order to arrive at an optimal moderator combination which well satisfies the needs of all instruments. The number of moderators on the SP target station will be an important issue to address, and for example an enhanced area moderator will probably make most sense if it replaces 2 moderators of the original 4 moderator concept. If there is a real need for poisoned moderators is a question to be specially examined in view of point e) above and the capability of mechanical choppers to produce shorter and nicer shape pulses for thermal and cold neutrons. Two moderators per target station (with 2 viewed surfaces each) would allow to place all moderators to the most brilliant position and it appears therefore to be a desirable solution.

Tasks and Schedule

It is obvious, that both the reference instrument suite and the reference design options of individual instruments will constantly evolve until design decisions will have to be gradually frozen on the time scale 2005 – 2007. The reference time line for ESS (assuming a decision on funding by 2004) calls for a start of commissioning in 2010 and user operation with about 20 "day one" instruments at a power approaching the nominal one in 2012. In the sequence of commissioning milestones, this schedule is expected to imply the start of neutron scattering research on the LP target station in 2010 at a power level of at least 1 MW, which will already make it the most powerful cold neutron source in the world. On this kind of time scale the priority scientific fields and goals will evolve and innovations in instrumental concepts and tools will emerge. Our immediate task is to elaborate and analyse a "day one" instrument suite which is the best that can be conceived on the basis of today’s scientific needs and technical state-of-the art (including all known innovation potential). It will then constantly upgraded to until construction decisions need to be made. Therefore it is crucial, that our study of the now proposed instrument suite also includes the evaluation of new, innovative instrument design options, concepts and tools to best satisfy the science objectives behind the currently proposed suite. In addition emerging, totally new experimental approaches might open up research opportunities, which cannot be foreseen today. There are two slots left in the first reference instrument list for such instruments, and new ideas are particularly encouraged and welcome. An incomplete, random list of already proposed innovative concepts to be considered as options (part of which are being or getting prepared for experimental test and/or prototyping): dynamic phase space transformation, neutron beam bunching by magnetic fields, refractive neutron lenses, focusing mirrors, focussing Bragg optics, repetition rate multiplication, wavelength band multiplication, pulse shaping choppers, adjustable resolution chopper systems, supermirror optical beam delivery system, ballistic neutron guides, spin echo for SANS and reflectometry, zero field spin echo approaches, etc.

Data acquisition, visualisation and evaluation will be of decisive importance. Existing neutron detectors would not be able to handle the counting rates (we can expect peak instantaneous counting rates for 1 cm^2 detector area up to about 100 kHz and 100 MHz in time average for an instrument.) Important and innovative detector development programs are in progress at many neutron scattering and other particle beam facilities and at university research groups, and it is fully reasonable to assume for our considerations in the Instrument Task for the time frame 2001 – 2003 that the detectors we will need will indeed be available by 2010 – 2012. On the other hand, it will become essential to add detector development to the ESS core activities by about 2004 and beyond. There is no doubt about the availability of the required computing hardware, and we have to be conscious of the huge potentials and needs in software development. While it is much too early to actually start developing software within the ESS project activities, it is important to prospect the new opportunities rapidly developing information technology will offer for smart data collection, evaluation and interpretation, both in terms of speed and depth. This has to be part of the ESS vision in instrumentation right from the beginning.

In order to proceed, we would like to ask the convenors to consult within the instrument groups which instrument(s) from the reference suite the group wishes to work on. Many people expressed interest at the various centres to join this effort and the groups might also interested to be extended/reconstituted.

The extended/reconstituted Instrument groups are asked to provide in a first iteration options for specifications, layout, choice of target station and moderator for the various instruments in the reference suites by 6 January 2002 by e-mail to Thomas Gutberlet (gutberlet@hmi.de). We will work out a synthesis of these first proposals and provide feedback from a global facility point of view for a review of the first iteration. Reasonably detailed design studies of the instruments considered will have to be completed in a preliminary form by end of February 2002 in view of presenting a report at the ESS-SAC workshop in 14-17 March 2002 near Paris, France. In order to discuss the feedback from this meeting and to launch the preparation of our final report for the European neutron User Meeting and the official presentation of the ESS project 15-17 May 2002 in Bonn, Germany, we suggest to have a 2 days meeting of the whole Instrument Task Group just after the ESS-SAC workshop, i.e. 18-19 March in Grenoble, France.

Thank you very much for your contributions, past and to come, to making ESS a decisive success. With best regards

Feri Mezei, Roger Eccleston, Thomas Gutberlet

ESS Day One Reference Instrument Suite
Version 1, 15. Nov. 2001

Note: Two instrument definitions in the same line tentatively suggests that one instrument might eventually successfully cover the two tasks. This suggestion needs to be examined. Polarized neutron option should be considered wherever major impact is to be expected.

- High resolution powder diffractometer
- Chemical single crystal diffractometer
- Small crystal protein diffractometer
- Magnetic powder diffractometer / Liquids diffractometer
- Engineering diffractometer.
- Single pulse diffractometer
- High resolution reflectometer
- High intensity reflectometer
- High intensity SANS
- Very low q SANS (10^{-4} $Å^{-1}$, focussing)
- Thermal chopper spectrometer / High energy chopper spectrometer
- High resolution cold neutron chopper spectrometer
- Variable resolution cold neutron chopper spectrometer
- High resolution back-scattering spectrometer
- High resolution NSE spectrometer
- Wide angle NSE spectrometer / Polarized neutron diffuse scattering (D7 – type)
- Tomography / Radiography
- \+ two novel instruments
- \+ instrument test facility