2017 Review of the Instrument Suite for Inelastic Scattering:

Chemical Spectroscopy Review

Committee:

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1. General Comments

The three instruments under review - BASIS, VISION and the Neutron Spin Echo (NSE) beamline - are all productive spectrometers in high demand. All three instruments are in good shape and running smoothly. The detailed evaluation includes a comparison of performance and productivity of each instrument and can be found in the following chapters. All three instruments are unique within the SNS and HFIR instrument suite and thus do not show overlapping capabilities. For VISION and BASIS this holds even true for the North American continent as no other quasi-elastic instrument or vibrational spectrometer, respectively, exists with comparable performance.

The alignment with ORNL and DOE missions is reflected in user proposals by ORNL staff as well as proposals on DOE topics of interest. Furthermore, part of the discretionary beamtime of VISION is being used for ORNL science initiatives through internal collaborations and strategic program development. NSE, being operated by Jülich Centre for Neutron Science (JCNS), is not as closely integrated in the ORNL operation making this alignment with ORNL and DOE missions less straightforward. Since JCNS will stop supporting the NSE instrument in 2020, the committee strongly recommends assessing the future possibilities for this instrument and its role within the DOE/ORNL mission as soon as possible to ensure a smooth transition in 2020. Further discussions can be found in the section on NSE.

It was noted that the beamtime allocation across all three instruments is not as effective as it could be. The committee suggests increasing the flexibility in scheduling beamtime and streamlining the safety reviews to fully optimize beam usage. It is duly noted that a rapid access mode exists at SNS, however this rapid mode still takes too long to be truly flexible. We suggest generating “super”-rapid access for time-sensitive measurements that cannot easily wait a few days. It is also highly beneficial for the productivity of the beamlines to allow for more discretionary time for proof of principle experiments and general testing. Discretionary time can also successfully be used to complete missing datasets for experiments that got cut short due to loss of beam or malfunctioning equipment. The completion of experiments often leads from an unusable dataset to publishable data.

Sample environment equipment for the three instruments is developing well. This needs to continue to keep the scientific impact of the experiments up and to attract new users from areas of science currently not using neutron scattering. The degree of integration of modelling and data analysis efforts into the beamlines varies among the three instruments. This effort should be continued and further improved. More detailed discussions can be found in the sections below.

The development of the chemical spectroscopy suite to complement BASIS, VISION and NSE is strongly encouraged by the committee. We include detailed comments on BWAVES in the BASIS section, on BeFAST in the VISION section, and on NSE capabilities for ORNL in the NSE section. In summary, BWAVES allowing measurements over several orders of magnitude in exchanged energy with the same instrument, is a novel kind of spectrometer which will allow new types of experiments; BeFAST plays a critical complementary role to VISION to cover the high energy transfer range; finally, a high resolution NSE spectrometer at HFIR is fundamental for the needs of the soft matter community and is necessary for ORNL to provide access to dynamical processes taking place over large length scales and long timescales. For these reasons, these three spectrometers are deemed of the highest relevance.

2. Review for BASIS

Overall Rating: 1 (exceptional performance)
Brief comments for each of the following aspects of BASIS:

2.1 Scientific Mission and Impact: 1

BASIS is able to cover a relatively wide dynamic range with sufficiently high resolution. The corresponding time window is tens of picoseconds to nanoseconds – covering two orders of magnitude in the timescale. This unique capability of BASIS makes it exceptionally suitable to study diffusion, relaxations, and some very low-energy excitations – prevalent in many soft and biological materials, but also in some condensed matter systems.

2.2 Beamline Productivity: 1

BASIS is one of the most productive and most in demand instruments at SNS/HFIR. Its oversubscription ratio is among the highest. The number of publications has been steadily increasing over the last three years. Although BASIS is supposed to be a “slow” inelastic instrument by nature, its number of publication has reached an impressive number of 36 in 2016 (with several in high-impact journals), which is even comparable to some of the high-throughput instruments. This is largely attributed to the close collaboration and guidance of the instrument scientists on the data analysis and interpretations.

2.3 Leveraging of specific SNS/HFIR characteristics: 1

High neutron flux at the sample

2.4 Effectiveness of beam time use: 1

Overall, the use of the beam time is effective. Occasionally, the effectiveness is impacted by the long time needed for sample safety review as well as the inflexibility of beam time allocation because of government regulations. See recommendations below.

2.5 General User Program quality: 1

The user base of BASIS is diverse, covering a wide range of disciplines. The users are well educated on using QENS due to the noticeable involvement of instrument team in data analysis and interpretation. This is evidenced by the high productivity of the beamline.

2.6 Adequacy and reliability of software, sample environment and ancillary equipment: 1

Software is sufficient, while major upgrade has been planned in 2019.
The choice of sample environment is limited due to the special requirements to the instrument geometry. But the existing sample environment can satisfy the majority of the users.
Furthermore, the instrument team is proposing to develop polarization analysis capabilities, which could be a tangible game changer.

2.7 Future instrument science and development plan: 1

The instrument has two major development plans: 1) to improve the shape of the resolution function by coating the analyzers with cadmium; 2) to develop polarization analysis capabilities. The latter is of great value for condensed matter experiments and could also be highly desirable by the biological and soft matter community. Another significant impact would be the study of the transport of Li^+/Na^+ in battery materials, for instance.

2.8 Overall: 1

Overall, the review panel highly praises the success and productivity of BASIS as well as the competency of the instrument team. It serves as a great example of a beam line of excellence. It does the best in the world in the unique time and length scales. To bring the instrument to the next level, we make the following recommendations.

2.9 Recommended Actions

1) Continue to refurbish the Si(111) detector tanks (2 of 4). The instrument scientist has already replaced one detector bank and shown that the resolution function has been significantly improved. This improvement can better the quality of data close to the elastic line for weak scatters or samples with slow dynamics.
2) Finish testing the BWAVE prototype (roughly $150K, 1 week of beam time). This work is critical to the strategic plan of STS. A successful demonstration of the concepts presented in the design of BWAVE is critical to ensure the preeminent leading role of ORNL in QENS/INS.
3) More effective beam time use could be achieved by the following:
   a) Increase the flexibility of the use of the beam-time, such as changing experimental plans or samples on the fly, contingent upon the approval of the instrument team and the safety team. Flexibility in adjusting the use of beam-time within the frame of the user program is necessary to run an instrument more effectively.
   b) Having safety review streamlined and extend the period of safety review validity.
   c) Allow more discretionary time for proof of principle experiments, testing, finishing experiments. Allow “super”-rapid access to allow time-sensitive measurements.
   d) Continue to improve ancillary equipment such as the polarization capability.
4) Hire one extra staff member to assist modeling and simulations. This could potentially lead to publications with even higher impact.

3. Review for VISION

VISION is the instrument for neutron vibrational spectroscopy located on BL-16B at the SNS. Neutron vibrational spectroscopy (NVS) uses neutrons to probe molecular vibrations which in turn provide information about chemical bonding, molecular structure, and inter- as well as intramolecular interactions. RAMAN and FT-IR spectroscopy are used to explore the same interactions with light instead of neutrons. As these two techniques are used in many laboratories world-wide among a large group of scientist, NVS is as easily approachable even for researchers in fields of science that do not commonly use neutron scattering. NVS has several advantages over optical spectroscopy such as its high sensitivity to hydrogen, the absence of selection rules and the easy-to-calculate neutron-nucleus interaction that allows quantitative simulation of the vibrational spectra. Additionally, neutrons can penetrate even bulky sample environment equipment easily.

3.1 Mission and Impact 1

VISION is an inverse-geometry instrument dedicated to neutron vibrational spectroscopy. It covers a dynamic range of roughly 1000 meV (or 8000 cm^{-1}), with the commonly used energy transfer range from -2 meV to approximately 500 meV. It operates at 30 Hz to include the elastic line in the measured spectrum. VISION is unique to ORNL. It is currently one of only two operating neutron vibrational spectrometers worldwide collecting data in this dynamic range with no required adjustments. VISION is world-leading for flux and has excellent resolution ($\Delta\omega/\omega$=1.5% above 5 meV), surpassing easily the only other neutron vibrational spectrometer TOSCA@ISIS.

Thanks to the high flux, many measurements require minutes rather than hours, especially with hydrogenous samples. This opens up the possibility of in-situ, time-resolved studies (e.g., catalysis or conventional chemical reactions) and revolutionizes the use of NVS instruments. This feature makes this instrument appealing to industry as batch processing and observation of reactions under realistic conditions is now feasible. The high flux also allows performing measurements on small sample sizes. The use of diamond anvil cell techniques on inelastic beamlines in the GPa range is now possible for the first time. For the same reason, measurements of non-hydrogenous samples have started to become routine on VISION as the flux is high enough to measure elements with small scattering cross sections, for example, observing CO_2 capture on surfaces.

VISION is unique within the SNS and HFIR instrument suite and only one other vibrational spectrometer with comparable properties in operation (TOSCA@ISIS). VISION's impact is clearly shown by a significant oversubscription rate as well as the number of users from overseas travelling to SNS to use VISION.

3.2 Beamline Productivity 1

VISION is not at its peak of publications yet as it is still a young instrument, having entered the user program in commissioning mode in 2014. The number of publications is steadily increasing from 7 in 2015 to 20+ for the 2017 runcycle at the time of writing. It already has shown its potential to become a workhorse instrument by the numbers of completed experiments per runcycle being close to 50 with VISION being still upgraded (technical quality factor 0.6). All indications are that VISION will move towards exceptional productivity over the next few years. This is due to the instrument's remarkable performance and to the dedicated support of the instrument team to the users in all aspects of their experiments. The support ranges from help with practical issues such as the preparation of the beam time proposal and the experiment, the sample treatment in the laboratory and the experimental setup, to the design of novel sample environment equipment and guidance during data acquisition. Data reduction, data analysis and modelling are also supported at the beamline during the experiment and following the return of the user to the home institution. The density functional theory and molecular modelling support for data analysis is a service to the user to provide the necessary data interpretation to finalize publications. This greatly reduces the time it takes to produce publications. The timely analysis of the data increases the impact factor of the publications. This support exemplifies the right way to keep the beamline productive, complete experiments successfully and publish high-quality data.

VISION shows how an exemplary combination of experiment and theory that can aid the user community in producing high-level publications. The current staffing level is too low to sustain this excellent support long term. The need to hire one more staff member for the experimental support is clear.

3.3 Leveraging of specific SNS/HFIR characteristics 1

VISION uses two pulses from SNS FTS to achieve its full energy range from -2 to 1000 meV. The short pulsed source and the brightness of the water moderator give this instrument the unmatched high flux. VISION is predicted to exceed its competitor VESPA@ESS on a bispectral, low-dimensional moderator (currently in design with hot commissioning planned for 2023) in the medium to high energy transfer range (>160 meV / 1280 cm^{-1}) albeit having less flux at lower energy transfer. This suits the scientific profile of the VISION scientific program well. See also "general user program quality".

3.4 Effectiveness of Beamtime 1.5

Overall, the use of the beam time at VISION is effective and idle time is minimized as much as possible. The instrument team is working actively to ensure that as little beam time as possible is wasted. Occasionally the effectiveness is impacted by bureaucratic issues:

- The beam time allocation at SNS is done in units of days. As VISION pushes the envelope with having extremely short run times for hydrogenous samples, the user office software should allow allocation in units of hours rather than days to make it possible to run several short experiments in one day. As flux increases at neutron facilities, this concern will become more common and should be addressed.
- The committee feels that there needs to be significantly more flexibility in adjusting beam time "on the fly" to take advantage of instrument idle time. The oversubscription

rate on VISION is high (factor 2-3) and any available hour should be used. Due to the generally quite short run times, even brief downtimes with one experiment ought to be used to progress with data collection for another (past or upcoming) experiment.

- This flexibility also needs to address the fact that beam time from a temporarily "idle" experiment (e.g., when a few hours are required to process a sample ex situ before continuing with a measurement) often comes unpredictably and sometimes at times when administrative staff needed to approve experiments is not available. There are several possible ways to deal with this. Beamline personnel should be given the responsibility and authority to decide (within established limits) what sample/experiment to run; or enough experiments presenting no significant hazards could be approved at the beginning of a run cycle to allow the instrument team to run the sample at any point in time during the current run cycle; or lists of previously approved samples could be maintained.
- The current fast access process is still too slow and too cumbersome to meet the needs of users in fast moving areas of research. Generate “super”-fast access to be able to run experiments immediately should there be time available.

3.5 General User Program Quality 1

VISION has a very diverse user community. This is one of the great strength of this instrument as it draws its user base not only from chemistry and physics but also from other research areas currently not that commonly involved in neutron scattering: geosciences, pharmacy, environmental sciences, and others. VISION is a potential gateway beamline at SNS to expand the neutron user community among non-traditional users. This wide user basis also implies that suitable sample environment equipment and laboratory space need to be available to meet the needs of such users.

Over the past three years VISION has made a great impact in showing vibrational spectroscopy with neutrons applies not only to static samples but also to in-situ, dynamic measurements. The common features of many VISION user proposals is that their experiments are related to chemistry or materials in general and as such often require sample preparation (e.g. gas adsorption on materials or synthesis of instable samples), sample treatment (e.g. activation of catalyst) and sample characterization before, during and after the experiment. To maintain performance the infrastructure for sample preparation and in-situ experiments, i.e. laboratories and sample environment, has to be continuously developed to meet arising needs.

While VISION currently already has four industrial collaborations, outreach will likely increase this number. The committee is very supportive of having the industrial proposal being non-proprietary so the results are published in peer-reviewed journal and boost the instrument publication list. So far the impact on environmental sciences and pharmacy is low and could be increased.

VISION is one of only two chemical spectroscopy instruments currently available to the user community at spallation sources worldwide (VISION@SNS,US; TOSCA@ISIS, UK). VESPA@ESS (Sweden) will come online in five years with a main focus on slightly lower energy transfer range than VISION. Even with VESPA@ESS initiating operation in 2023, beam time requests by the user community will not be satisfied by having only three neutron chemical spectrometers worldwide. More importantly, VISION exceeds TOSCA in flux in orders of magnitude allowing for very fast acquisition times permitting for the first time to perform true in-situ experiments on the minute scale which is of great interest to the catalysis community. It also allows measuring non-hydrogenous samples opening up the instrument for attractive research fields as CO_2 sequestration or ion conductors. Furthermore, the capability to measure small sample amounts on the scale of a few milligram enables techniques such as high-pressure measurements using anvil techniques. The achieved pressures in the GPa range are not common for inelastic instruments and open up yet another field of research. High-pressure measurements might also make it possible to measure "soft" materials with a large Debye-Waller broadening of the vibrational peaks at room temperature to be measured at temperatures of 300K and above while under pressure.

3.6 Adequacy and reliability of software, SE and ancillary equipment 1

VISION was the first beamline at SNS to convert data acquisition and instrument control to the Control Systems Studio software (CSS). Various dedicated Python scripts developed by the beamline team allow users an easy and fairly intuitive access to instrument control and data acquisition. Beyond automatic data reduction at VISION, there are user-friendly Python scripts for MANTID for data manipulation. Most users return to their home institution with reduced and (at least) partially analyzed data. The VISION team performs standard density functional theory (DFT) and molecular dynamics (MD) calculations during the beam time as a service to users. These calculations run on a dedicated computer cluster (the Virtues cluster). This novel, unique, and highly successful approach greatly boosts productivity at VISION. It will likely be emulated by other instruments at SNS and elsewhere as the cost of computer clusters continues to decrease.

VISION's core sample environment is the closed-cycle helium refrigerator that cools samples and sample environment equipment. There are several specialized sample sticks and sample cells available to the users. These reflect the current demand of science: gas loading/gas flow, pressure cells, electrochemistry, high temperature, or in-situ Raman scattering. Ancillary equipment such as a dedicated gas panel, the ortho-para converter and the impedance spectrometer are also available. The sample changer that is currently being installed and tested will make a mail-in program feasible for VISION as well as boost the productivity of the instrument by batch processing of reference samples or screening of materials.

VISION is in very good shape and should continue to develop sample environment capabilities with the emerging new science interests of an ever expanding group of users. The need for expansion holds equally true for timely access by (short term) neutron users to a well-equipped chemistry laboratory to synthesize and characterize samples. The current access that has been achieved over the past 3 years is getting better, but more equipment and space for sample characterization will be needed as experiments and samples continue to grow in complexity. The laboratory space should grow accordingly. SNS trails other facilities in terms of sample preparation and characterization space and capabilities.

3.7 Future instrument science and development plan 1

VISION's immediate development plan has been well presented by the instrument team. They need to finish commissioning the sample changer and finish installing the diffraction banks at 90 degrees to allow crystallographic phase identification while measuring NVS. Diffraction should become a standard tool for the VISION users when measuring non-hydrogenous samples.

The procurement of a CCR with a larger sample chamber will allow more flexibility for using complex sample environment in the CCR as the size constraint is relaxed compared to the current CCR. This is a step towards unlocking new scientific capabilities as new sample environment equipment can be used on VISION (e.g. magnets or larger pressure cells). As long as VISION can keep developing sample environment and sample preparation capabilities to match the science that is being proposed, it will easily stay ahead of possible competitors such as VESPA@ESS.

3.8 Overall 1

VISION is currently a unique and a very impressive instrument to use. There are many new possibilities to explore with NVS that were not accessible before on instruments with less flux. VISION is a well-run instrument that given the right amount of support (personnel) and investments in sample environment will be leader of its class for years to come.

The **overall rating** for VISION is 1 (exceptional performance)

3.9 Recommended Actions

1) ORNL should hire a third instrument scientist with chemistry or related scientific background and good experimental skills to assist users with the practical part of the experiments. Thanks to the high flux, spectrometers like VISION are now becoming high-throughput instruments that are attracting users with more and more complicated setups and in-situ or time-dependent runs. This requires expert assistance for the users in the preparation of the more complicated experiments, as well as help in evaluating data as it is acquired to make decisions on the spot regarding the course of an experiment. With run times of the order of minutes to a few hours, the current level of staffing is not enough to cover user support 24/7 during a run cycle.
2) VISION urgently needs more dedicated laboratory space housing sample characterization equipment (such as BET, FT-IR, XRD, TG/DSC ….) to investigate changes in samples before/during/after beamtime as well as check samples that are synthesized at SNS because they cannot be transported easily. As a start two actions could be taken: a) the chemical fume hood in the VISION lab needs to be installed to allow for handling of chemicals in this laboratory located close to the beamline and b) more space in the chemistry laboratory

area on the 2nd floor of the main office building at SNS needs to be claimed to house more equipment supporting SNS (and VISION) users with more sophisticated sample handling needs.

3) VISION needs a custom-made CCR with a larger sample compartment to accommodate bigger sample environment equipment. This will open up scientific areas that are currently difficult or impossible to approach, e.g. using magnets or larger pressure cells.
4) ORNL should build BeFAST on beam port BL-16A to complement VISION in the high-energy range. Easy to build and operate it will make effective use of the small space between VISION and NSE. BeFAST can supply users of neutron vibrational spectroscopy with the information on stretching modes of molecules, an energy range where VISION has more limited intensity and resolution. Besides complementing VISION, BeFAST will ease the oversubscription at VISION, especially for experiments requiring poorer energy resolution.
5) The 90 deg. diffraction detector banks must be installed together with the necessary collimators. The corresponding data reduction software must be developed.
6) User community development efforts ought to be encouraged and supported (workshops, conferences, seminars, etc).
7) Simplify the beam allocation/run authorization process to take advantage of the flexibility afforded by the VISION high flux, which permits the interleaving of experiments for increased efficiency and productivity.

4. Review for NSE (Neutron Spin Echo)

Neutron Spin Echo (NSE) spectrometers use the Larmor precession of the neutrons' magnetic moment in the magnetic field created by two large solenoids, one placed before and one placed after the sample, as an internal clock to determine the change in velocity of the individual neutrons due to the scattering process. This method allows one to obtain the highest energy resolution possible (sub μeV) over a wide range of incident wavelengths. NSE instruments directly measure the real part of the intermediate scattering function, I(Q,t) (where in the context of NSE measurements t is commonly referred to as Fourier time), i.e. the cosine Fourier transform of the scattering function S(Q,ω), and is used to study slow dynamics found in condensed matter systems.

Among the neutron scattering spectrometers, NSE covers the largest length-scale (with Q value as low $\approx 10^{-2}$ $Å^{-1}$) and the longest time scale (100s ns). They afford unique capabilities which are exploited in a number of fields, such as soft matter, biology, chemical physics, and magnetism. Among these fields, the NSE spectrometers have traditionally been most successful for soft condensed matter and bio-related study; however, also in chemical physics and magnetism, NSE provides unique measurement capabilities and has specific niches of interest.

The NSE spectrometer on BL-15 at SNS has been operated by the Jülich Centre for Neutron Science (JCNS) since 2010. The current agreement between the JCNS and ORNL for the operation of the SNS-NSE expires in 2020 and is not clear how the operation of the instrument will be managed afterwards.

4.1 Scientific Mission and Impact 2

The role of the SNS-NSE is to complement the suite of spectrometer at ORNL to afford the possibility to investigate a Q range (down to $\approx 10^{-2}$ $Å^{-1}$) and time range (up to ≈100 ns) unattainable with other instruments. There are only two NSE instrument operating in North America and currently only 4 Mezei type instruments worldwide. Within this context the SNS-NSE plays a strategic role responding to specific needs of the scientific community. In fact, the SNS-NSE is significantly over-subscribed.

4.2 Beamline Productivity 2.5

Experiments on NSE last on average 7 days, hence the throughput of these instruments is not very high. A rough average of the productivity of other NSE instruments worldwide gives 8-10 publication/year. Over the last four years the SNS-NSE publication record averages out to 6.5 papers/year. However, the productivity varies significantly from 4 publications in 2016 to 11 in 2017. The overall performance is below the worldwide average and is not fully satisfactory. Moreover, a few publications in high impact journal notwithstanding, the average impact factor of the published papers should also improve. On the other hand, the results of 2017 indicate that the instrument has the capability to provide the expected output. Moreover, there is a clear upward trend from 2010. Looking more closely at the publications, it is clear that high quality data can be collected on the SNS-NSE. At least a couple of very challenging experiments, i.e. grazing incidence NSE measurements, have been successfully carried out. The most successful work requires (and has been carried out with) significant investment of resources. NSE uses significant amounts of sample, and deuteration is needed. Interpretation of the data often involves modeling efforts either through calculations or computer simulation. These requirements often become a significant barrier to new users. However, expert users and users at ORNL have access to such capabilities. It would be beneficial for the NSE program to leverage in house opportunities. Future strengthening of the ORNL soft matter community will benefit NSE; in turn, NSE will provide unique capabilities to a still developing community.

In summary, the SNS-NSE beamline productivity has not plateaued, yet. Publications number and quality are improving. Recent high impact publications have appeared which have the potential to stimulate and broaden the user base. However, a continued effort supporting the instrument and developing the user community will be required in order to continue improving. The goal is a steady production of high impact work.

4.3 Leveraging of specific SNS/HFIR characteristics 3

The SNS-NSE is the only spin echo spectrometer operating on a spallation source; whether this represents an asset or a significant shortcoming is not easily answered. On a continuous source NSE operates with typical $\Delta\lambda/\lambda \approx 15$ %, which affords high neutron flux on the sample (in spite of the high energy resolution of the instrument), the Q and t values being varied by changing the second arm position and the precession field intensity; at SNS, the NSE operates using wide energy bands, e.g. $5.9 < \lambda$ (Å) < 9, covering a wide Q and t range for the same arm configuration and precession field intensity. The different modes of operation are in principle equally efficient; however, running in the time of flight mode requires additional care in the measurement planning. As judged by the performance of the SNS-NSE compared to other instruments, operating on a pulsed source cannot be considered a major disadvantage, the situation might however be different depending on the specific experiment. On the other hand, the time encoding affords unique possibilities in terms of Q resolution as compared to reactor based NSE. It could be envisioned that such capabilities could be relevant to avoid detrimental effect from Bragg peaks and hence be useful for chemical physics and magnetism related studies; however, it does not seem like this possibility has been fully explored by the users so far.

A crucial parameter is the usable wavelength range which currently seems to be limited up to ≈11 Å. It is not clear, whether this limitation is due to the characteristics of the polarizer or of the source and hence whether it could be overcome. However, the maximum usable incoming wavelength determines the maximum Fourier time achievable (which scales with λ^3) and currently prevents the SNS-NSE to attain Fourier times of several hundreds of nanoseconds. Other instruments worldwide do currently offer the possibility to measure Fourier times longer than 200 ns or could be envisioned to do so. In this respect, a comparison to the potentialities of a NSE spectrometer at HFIR is relevant and will be discussed in the following.

4.4 Effectiveness of beam time use 2

Because the duration of a NSE experiment is rather long (on average ≈7 days) the number of experiment performed is not high compared to other instruments. Moreover, the SNS-NSE gives 25 % of its beam time to the Jülich Centre for Neutron Science, a quota which is outside the user program. The effectiveness of the beam time use is adequate. However, given the small number of experiment performed each year it is crucial that unfeasible experiments will be screened out. Moreover, all experiments and in particular the more challenging ones should be allocated sufficient time. Instrument productivity would improve by further development of current avenues for experiments feasibility testing and quick access for finalizing studies.

4.5 General User Program quality 2

The SNS-NSE has been operating within the ORNL user program for several years now. The user program operation has reached maturity. However, although the instrument is highly oversubscribed, further development of the user community should be a target. Outreach exercise would be beneficial. Also important would be the development of an expert user community within ORNL. Further strengthening the support for neutron users already provided by ORNL in terms of deuteration and computing facility with a specific focus for NSE could also significantly help developing the quality of the SNS-NSE user program.

The use of NSE for magnetism studies is not fully developed. Suitable Q-coils for full polarization analysis have only recently been developed. Some deficiency in terms of sample environment will be discussed in the following. The number of suitable NSE experiments in magnetism should not be expected to be large but a niche area exist which has not been fully tapped upon, yet.

The uncertainty regarding the future of the SNS-NSE after 2020 might soon start to negatively affect the user program.

4.6 Adequacy and reliability of software, sample environment and ancillary equipment 2.5

The instrument control software is adequate; however, it is not user friendly; given the slow turnaround of NSE experiments and the strong support from the NSE team, this does not represent a significant issue, there is however room for improvement. The current data reduction software echodet, although properly functioning, is not fully satisfactory. Echodet has been developed and is still mostly maintained by M. Monkenbusch. Echodet is not user friendly; moreover, when issues which cannot be addressed without the help of M. Monkenbusch arise, solving these problems can become cumbersome. A new data reduction software, DRSPINE, has been developed by the SNS-NSE team but it is still not widely available to the users. Such effort should be supported. Given the flexibility of the SNS-NSE data grouping, the employment of DRSPINE has the potential to significantly improve the productivity of NSE.

Sample environment and ancillary equipment are generally adequate but there is also room for improvement. Cryostats reaching sub Kelvin temperature which could be required for magnetism experiments are currently missing.

The on-going effort to develop new sample environments such as for example the Electric Field Cell, Light Cell, and the High-Pressure Cell are commended, could open new opportunities, should be supported as much as possible within the current agreement with the Jülich Centre for Neutron Science.
The aging of the current power supplies is a significant concern. Precautionary actions are needed. The adoption of newer technology currently employed for the J-NSE instrument at FRM-II could be a possible solution.

4.7 Future instrument science and development plan N/A

Recent improvements in the design of NSE precession coils allow to reach maximum field integrals (notice that the Fourier time is proportional to the field integral) of ≈1.1 T·m which is significantly higher than what is currently available at SNS-NSE (≈0.5 T·m, notice that the SNS-NSE was initially designed to reach a maximum field integral of ≈1 T·m). Such developments have successfully been tested on both IN-15 at ILL and at the J-NSE at FRM-II. These improvements allow to measure up to 200 ns using 10 Å incoming neutrons which is more than double what currently available at SNS-NSE with a similar wavelength band. With the use of incoming wavelengths of $\lambda > 15$ Å, Fourier times of the order of several hundred nanoseconds are achievable. This significantly extends the available time range and opens new scientific opportunities. It would be a severe limitation if ORNL would not provide a similarly wide available dynamics range to its user community. An entire range of scientific research in soft condensed matter on systems as diverse as polymers, nanocomposites, complex systems, membranes, and other bio-related materials could not be carried out at ORNL. However, providing the possibility to cover a dynamic range up to several hundreds of nanoseconds is not achievable by ORNL without significant investments. Currently, the SNS-NSE can only reach ≈150 ns. Improvements of the correction coil technology are possible but there is no guarantee of success. The adoption of optimally designed precession coil could allow to reach comparable field integrals to what is currently available on IN-15 and J-NSE. However, the maximum Fourier time achievable will be still limited by the range of incoming wavelength realistically usable.
Building a NSE spectrometer at HFIR after the Be reflector change and redesign of the cold neutron guides system would guarantee a straightforward path to allow ORNL to offer to the user community coverage of a dynamic range in Q and t at least as wide as achievable in other facilities. The unparalleled flux of HFIR would ensure to have a world class NSE instrument. The possibility to use incoming wavelength as long as 20 Å with a significant flux would allow to reach very long Fourier times. Hence the NSE at HFIR affords ORNL a unique possibility to have a leading high resolution NSE spectrometer.
With a high resolution NSE instrument at HFIR the role of the SNS-NSE will change. It is hard to imagine the SNS-NSE to be able to compete with the flux and the long wavelengths available at HFIR for the studies of long relaxation processes. It could be envisaged that the SNS-NSE could play a complementary role as it was effectively done by the IN-15 and IN-11 duo at ILL for several years. In particular, the SNS-NSE might be dedicated to chemical physics and magnetism investigation which do not as crucially depend on the maximum Fourier time and would benefit more from a wider angle coverage and the possibility to investigate higher Q values. Obviously,

so far, the SNS-NSE had a very different focus and such a change of direction might require even additional efforts and further instrument development.
As an aside, in the discussion of complementary instruments to a high-resolution NSE at HFIR, the possibility of a WASP type instrument on the STS has been also envisaged. Given the number of unknowns it is however beyond the scope of the present document to discuss it.

4.8 Overall 2.5

The neutron spin echo spectrometer at SNS respond to a specific need of the neutron scattering community to study long relaxation processes over times scales of the order of tens of nanosecond and length scales of the order of tens of Angstrom. The capabilities of the instrument are comparable to those of other machines worldwide. The output of the instrument is not fully satisfactory yet but is improving. At the same time, the user community has not fully developed yet and needs as much support as possible to flourish. Operation of the instrument is satisfactory but there are opportunities for improvements.

4.9 Recommendations:

1) ORNL should commit to the long term support of the SNS-NSE as soon as possible. The uncertainty regarding the long term status of the instrument might undermine instrument operations, discourage a still developing user community, and sap the NSE team moral.
2) The efforts to support the soft-matter user community, both within and outside ORNL, should be continued. Providing both deuteration and data interpretation support (via suitable computing facilities and personnel) specifically tailored for NSE users could be beneficial.
3) The new reduction software DRSPINE should be deployed as soon as possible. Current new sample environment development projects should be supported without forgetting the need of the magnetic community. The staffing of the NSE team should be shored up. A plan for timely replacement of the aging instrument components should be devised.
4) Current avenues for experiment feasibility testing should be expanded.
5) The project of a high resolution NSE spectrometer at HFIR is highly recommended as the best avenue to provide the user community with the possibility to study relaxation processes of the order of hundreds of nanoseconds. This dynamic range is crucial for the soft-condensed matter field. Studies should be started regarding a possible complementary role played by the SNS-NSE alongside a high resolution NSE spectrometer at HFIR.