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TITLE: SCATTERING KERNELS AND CROSS SECTIONS WORKING
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International Workshop on Cold Moderators for Pulsed Neutron Sources

Scattering Kernels and Cross Sections Working Group

Gary Russell, Chairman and Bob MacFarlane, Co-Chairman

**Torben Brun, Lowell Charlton, Laszlo Cser, Jack Dorning,
Phil Ferguson, Tony Gabriel, Rolando Granada, Erik Iverson,
Hans Ludwig, Dave Picton, and Bob Williams**

Summary and Action Items

• Immediate Needs of the Cold-Moderator Community and How to Fulfill Them:

- The cold moderator scattering kernels of Bob MacFarlane¹ represent the "state-of-the-art" kernels for direct use with MCNP.
- On the near-term (early 1998), Los Alamos will make available its most recent set of cold-moderator scattering kernels to the Cold Moderator Workshop participants. On the long-term (August-September, 1998), Los Alamos will work to get a quality-assured version of the kernels to RSIC for a wider distribution. Until then, Los Alamos would not like the kernels redistributed by the workshop participants.
- Scattering kernel data will be processed for the following materials and temperatures:
 - Liquid H₂ at 15, 20, 22, 26, and 30 K,
 - Liquid CH₄ at 90, 100, and 110 K, and
 - Solid CH₄ at 22, 26, and 30 K.

• Synthetic Scattering Kernels:

- The synthetic scattering kernels of Rolando Granada for liquid and solid CH₄ should serve as good benchmark checks for Bob MacFarlane's methane kernels.
- The synthetic kernels allow the possibility of generating scattering kernels for other potential cold moderator materials (within the constraints of the assumptions used). It would be useful to incorporate the synthetic scattering kernels into MCNP. However, no one has been identified to do this work.
- Gary Russell and Rolando Granada will work together to benchmark the synthetic kernels and MCNP kernels for liquid and solid CH₄ for simple problems.

• Very Simple Synthetic Scattering Functions:

- Jack Dorning conjectured that the use of *very simple* synthetic scattering functions holds promise to gain insight to time dependent neutron thermalization issues and to perform gross checks on Monte Carlo simulations.

- The techniques would employ very simple synthetic slowing down kernels and very simple thermalization kernels to carry out mathematical analyses of the slowing down, transport, and thermalization equations.
- No one was identified to carry out this work; nevertheless, this "hand made" physics should be done.

• **Measurements of Interest:**

- It would be useful to have the total cross section of ortho- and para-hydrogen measured at energies below 1 meV, with careful ortho/para concentration control.
- Additional measurements on cold-moderator materials are needed that would help validate the scattering kernels. For example, $S(q, \omega)$ and total cross section for liquid and solid methane and liquid H_2 in thermal equilibrium at several temperatures.
- At ISIS, it would be useful to measure the neutronic performance of their H_2 moderator in the liquid and supercritical states, and at various proton beam currents.

• **General Issues:**

- Torben Brun provided a number of references for measurements associated with Liquid H_2 for consideration in comparison with Bob MacFarlane's scattering kernel.
- Bob MacFarlane will compile data from anyone on other cold moderator materials and will distribute the information as appropriate.
- There is a need to resolve the question of the relative concentration of ortho- and para-hydrogen in a liquid hydrogen moderator in a radiation field. We also must come up with a viable scheme to measure the ortho/para ratio in real systems.
- Bob MacFarlane will devise a scattering kernel for lead. Other materials will be considered as time and funding are made available.
- The Bariloche group (Granada) is also able to produce synthetic scattering kernels for lead and other structural materials.²
- It was agreed to exchange measured moderator performance data and calculated predictions between ISIS, IPNS, Lujan Center, KENS, and Hokkaido University.
- The use of amorphous carbon fibers for a cold moderator was suggested. Such a cold moderator may be more attractive for a reactor source than for a short-pulse spallation source.

General Observations and Comments

Scattering Kernels

There was widespread agreement that Bob MacFarlane's latest scattering kernels are the best data available, and all workshop participants should have them. The angle and energy bin structures used for the kernel calculations are important, and Los Alamos needs to look at these details carefully.

Bob MacFarlane will act as a repository for experimental data on cold moderator cross sections, etc., and it is encouraged that people send this type of information to him. Bob will distribute the data as needed, and keep a catalog of references. He will prepare existing evaluations at multiple

temperatures and provide them to a limited number of people (i.e., the Cold Moderator Workshop participants):

Liquid H₂ @ 15, 20, 22, 26, and 30 K,
Solid CH₄ @ 22, 26, and 30 K, and
Liquid CH₄ @ 90, 100, and 110 K.

The time scale for producing these data sets is early in 1998. Los Alamos will validate and release a common set of cold moderator data. The time scale for this release is August-September, 1998.

Everyone should work to try and define what additional experimental results would be needed to try to validate or improve the scattering kernel physics models. The time scale should be within one year and Bob MacFarlane would act as a repository for these ideas.

Possible other future data sets (in order of likelihood and timeliness) are:

Be and Graphite @ 77 K
Pb @ 77 K and 300 K with inelastic and Bragg edges
Al @ 77 K and 300 K with inelastic and Bragg edges
CH₂ @ 15, 20, 22, 26, 30, and 300 K

It would be useful to have a mechanism to label the MCNP data sets that the various groups are using. It would also be beneficial to compare Monte Carlo results using the standard kernels and using simpler kernels given by analytic techniques and by simple physics to be able to understand what is going on and to provide checks on the numerical data. A suggestion is that the S(α, β) files get a release date based serial number (or some similar designation).

The cold-moderator community should converge to a common set of S(α, β) data files, to be created by Bob MacFarlane, which will include liquid H₂, liquid CH₄, and solid CH₄ at a variety of temperatures which are not outside the scope of the present physics models. The community should combine its findings for existing measurements of σ_t , $\sigma(E \Rightarrow E')$ and $d\sigma^2/d\Omega dE$ for all these materials, with the intent that the data can be compared to the predictions of the physics models. This would include strict attention to the ortho/para-hydrogen question in liquid H₂, which we still do not know how to reliably measure in situ.

Some consideration should be given to other materials, that is, solid CH₄ < 20.4 K, supercritical H₂, and all the other materials mentioned during the workshop - perhaps by the synthetic kernel formalism discussed by Granada. This would include the above "other" phases of present materials, as well as other materials like metal hydrides (perhaps non-crystalline), deuterated hydrocarbons, more complex hydrocarbons, and perhaps ammonia as well. This would of course, have to start with inelastic and elastic total scattering measurements.

Synthetic Scattering Kernels

Synthetic kernels show promise in the area of quickly evaluating new materials without the effort involved in our current S(α, β) evaluation scheme. We should test the synthetic kernels and determine if they should be used in the initial scoping work for new spallation source design.

The synthetic scattering function allows a simple description of the incoherent interaction of slow neutrons with hydrogenous materials. The main advantages of this model reside in the analytical expressions that it produces for double-differential cross sections, energy-transfer kernels, and total cross sections, which permit the fast evaluation of neutron scattering and transport properties.

Concerning cryogenic materials, the synthetic scattering function has been tested for liquid and solid CH_4 against available data, showing good agreement. In the case of liquid H_2 , the input data for the model should be revised in light of new information on the frequency spectrum; this may involve a proposal to perform a measurement of the double differential cross section, as well as the total cross section of para-hydrogen for neutron energies below 1 meV.

In particular, a precise knowledge of these quantities (σ_i for ortho- and para-hydrogen) at very low energies is needed if transmission measurements are going to be performed to determine the ortho/para ratio in a specific system. In the present situation, the capability (or difficulty) to establish that value seems to dominate the inaccuracies of present liquid H_2 kernels.

Gary Russell and Rolando Granada will collaborate on comparing neutron spectra for liquid and solid methane moderators for simple geometries using both Bob MacFarlane's scattering kernels and the synthetic scattering kernels of Granada's Bariloche group. The Bariloche team is exploring the possibility of including the synthetic model as an option in the NJOY system. It would be very useful if the formalism for synthetic kernels could be incorporated into MCNP to allow modeling of "non-standard" moderator ideas, i.e., hydrides, organics, etc.

Simple Synthetic Scattering Functions

Jack Dorning proposed that "simple physics" calculations could be done by hand (or almost by hand) to gain insight into the salient phenomena of cold-moderator thermalization. Also, such calculations would provide useful gross checks (i.e., "credibility checks") on the large-scale Monte Carlo calculations already being performed. Some ideas along these lines would be to carry out simple mathematical analyses of slowing-down equations, transport equations, and thermalization equations using "very simple" synthetic slowing-down kernels and "very simple" thermalization kernels. The use of these simple kernels would make the equations fairly easy to solve, and the analytical solutions or very simple computer-generated solutions would provide substantial physical intuition and insight as well as gross checks on the results of large-scale computer simulations.

The simple synthetic slowing-down kernels that could be used initially are those developed by Wigner (the Wigner kernel) and Goertzel and Greuling (the Goertzel-Greuling kernel) both of which correctly retain the total energy-dependent cross section and the average logarithmic energy decrement. The Goertzel-Greuling kernel also preserves the mean square lethargy increase per collision. More advanced "simple" slowing-down kernels, such as the one developed by Cadillac and Storrer (in which the energy spectrum of scattered neutrons can be included) also would be very useful. Finally, simple synthetic kernels developed for slowing-down by inelastic scattering, developed by Benson and others would also be advantageous.

Analogous simple synthetic thermalization kernels (such as those used by Nelkin, Corngold, Dorning, and many others) also could be used to do analogous thermalization calculations.

These kernels satisfy the detailed balance condition and can be made to correctly reproduce a energy-dependent total scattering cross section of the form

$$\Sigma_s(E) = a/v + b,$$

where b is the free atom cross section, of the form of the free gas scattering cross section, or of the form of any energy-dependent total scattering cross section. Which of these are used depends upon how close the physicist wants to mimic the physical system on the one hand, and how much time he has available to carry out the analysis of the resulting equations on the other.

Finally, the use of simple expressions for the asymptotic time-decay constant such as

$$\alpha_0 = \langle v \Sigma_a \rangle + \langle v D \rangle B^2 - C B^4$$

could be used as gross credibility checks on the large-scale Monte Carlo simulations, and other large-scale numerical calculations.

General Observations and Measurements

We need to resolve the question of the ortho/para-hydrogen ratio in a liquid H_2 moderator in a radiation field. Existing sources may be unable to measure the ortho/para ratio directly because of the resistance to the installation of invasive measuring devices. Therefore (at this time), we can only infer the ortho/para concentration (and behavior) from computational results compared to the measured neutron spectrum.

Are their gaps in the liquid H_2 kernels that contribute to the confusion? Perhaps there are, and we must continue to look into the details of the liquid H_2 scattering kernels. Careful measurements of the total cross sections for liquid para-hydrogen and liquid normal-hydrogen for low energy (< 1 meV) were suggested, with careful ortho/para concentration measurements and control. Differential liquid H_2 cross section data is nearly non-existent, and more measurements are sorely needed. For example, a $d\sigma/dE$ measurement of $J=0$ to $J=1$ cross section (para to ortho) would be a very valuable measurement to make.

If someone can perform such measurements, data for supercritical H_2 at low temperatures would be very useful to determine whether or not existing kernels are adequate for supercritical H_2 . (Note: this topic may have already been addressed by the reactor community and found not to be an issue.) It was suggested that measurements be made at the ISIS facility to verify this. Also, it would be useful to obtain neutron spectra from the ISIS liquid H_2 moderator as a function of proton beam power.

On the longer-term, more work needs to be done on liquid ortho- and para-hydrogen cross section calculations. There is a need for MCNP to be made more user-friendly for cold moderator calculations, e.g. to allow mixing of different $S(\alpha, \beta)$ scattering laws for the same nuclide. It was suggested that input parameters for "standard" moderators (liquid and solid CH_4 , liquid H_2 , etc.) be included in the MCNP user manual.

What improvements would be used to verify liquid hydrogen better? Some suggestions were: a) inelastic scattering from well-characterized sources; b) measurements on as-built moderators;

and use time-dependent measurements (e.g., long-time die away constants). It was noted that different operating liquid hydrogen moderator systems may vary in ortho/para-hydrogen ratios.

Perhaps, the primary problem in scattering kernels is the admixture of para- and ortho-hydrogen. In order to properly address the problem, the cross sections must be accurately known and the admixture at a given time in a liquid hydrogen moderator must be known. This is a long-standing problem not likely to be solved in the near term.

References

1. R. E. MacFarlane, "New Thermal Neutron Scattering Files for ENDF/B-VI Release 2," Los Alamos National Laboratory report LA-12639-MS (ENDF 356).
2. J. Granada, et al., *Annals of Nuclear Energy* **24**, 763 (1997).