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SUMMARY OF SESSION ON MODERATORS.

J.M. CARPENTER & G.J. RUSSELL

The afternoon of Tuesday was devoted to reports and discussion about moderators. We had five reports: one concerning the "Burping" of cold solid methane; another report on the operation of the LANSCE liquid hydrogen moderator system; another report on the operation of the ISIS cryogenic moderators; another concerning the way moderators deteriorate in performance under irradiation and another report in general about the LANSCE moderators.

Everyone seems to have troubles starting up these systems: we build them; we evacuate them; they are warm and we try to cool them off and fill them up with whatever liquid. Well, there's trouble. The general question that needs to be resolved is that of the stability of these (flowing) liquid methane and liquid hydrogen moderator systems. We need better understanding of how to control these systems, especially during the filling stage which requires of the order of 4 to 8 hours. It sometimes requires an experienced driver to coax the system from where it begins to where we want it to go.

Other questions, which we didn't discuss too much, are: how stable is the temperature of these moderators? How can we control the temperature of these moderators? Maybe we don't need to do anything. Some of the instrument people on the neutron beams say, "I want the moderator temperature to be held within 0.1K", just so they don't have to worry about it! No one that I'm aware of, keeps the moderator temperatures within 0.1K!

The following principal points were made in a discussion on the question of moderator temperature stability:

- *The change of temperature causes a shift of the Maxwellian and hence changes the spectrum shape.*
- *Spectrum shifts between fills of the methane moderator have been observed at ISIS, even though they go back to the same nominal temperature. This effect is not yet understood. It is not certain if this effect occurs also with hydrogen moderators, because only the type of instruments that look at methane moderators seem sensitive to the effect.*
- *The procedures to deal with these spectral shifts are believed to be straightforward; normalise everything to the monitor spectrum before you process the data, although it is not quite as straightforward as first appears because the monitor is not at the same position as the detector (rescale according to wavelength to make these corrections). There are also other problems (to match up resolution broadened Bragg edges, etc). Apart from being an extra thing to do, it also makes it substantially more complicated to do a 1% experiment.*
- *If the spectral temperature becomes unstable, it is possible to recover data. In the case of liquid hydrogen there is a much more severe thing that can happen; the pulse shape (distribution in time of neutrons of a given energy) may well change significantly if the ortho- to para-hydrogen ratio changes. There would seem to be no way of directly monitoring the ortho to para ratio, hence it is difficult to see how to have any ratio other than the stable value at a given temperature. The pulse shape change causes the resolution to change (probably at the "factor of two" level). One could probably monitor it with a crystal analyser and even though in principle one could recover the data, probably experimenters would just say, the source is no longer stable and wait until it's fixed.*

In these respects, I suppose, we are simply not serving the instrument people according to what they would like, but then they are probably making excessive requests - just now we are ignoring them! They (the users) more or less get along. Eventually we are going to have to accommodate them and provide some control.

There is the question of the temperature instability of solid methane that takes place upon intense irradiation at low temperatures (similar questions probably arise in cold D_2O ice systems). Although we are coming to understand these phenomena, there is a great deal more to learn. Certainly an unresolved issue.

We have several liquid methane systems operating but these are all more or less low power; so as ISIS comes up, we will be watching to see what happens to the liquid methane systems when they have to withstand higher dose-rates and higher power densities. Just now, the systems at IPNS and ISIS behave rather acceptably, but it remains to be seen how things behave at higher power densities.

There were several issues resolved in our discussions. We found out how room temperature polyethylene and solid methane deteriorates under irradiation. Probably a result of all that is that in higher power sources we won't use polyethylene ever again, just water. Solid methane is so attractive, that we will continue to use it; from what we know about how rapidly it deteriorates, we can determine a schedule for replacing it. The "Burping" phenomenon is approximately understood, although the thing is not quantified, worked out and controlled. We have operating liquid methane and hydrogen systems, so that we know that these are satisfactory at the present low powers. So we can count as a resolved issue, whether or not we can build and successfully operate these at low powers.

A wild idea surfaced: if we cannot use solid methane at 20K and if hydrogen has such a squirrely scattering kernel that you get a funny spectrum and you would like to do better than that, then how about combining these two in some fashion like circulating a slurry of solid methane suspended (although it doesn't float) in liquid hydrogen. I'm afraid that I must take the blame for this wild suggestion!

Gary Russell has agreed to talk a little bit about the next issue, so I'll just treat this very briefly. There's a body of data on spectra and pulse-widths as functions of temperature and poisoning etc. for polyethylene

and (liquid) water. The same is true for liquid methane. Furthermore, we have reasonably good scattering kernels and calculational methods which are now bench-marked for water/polyethylene and liquid methane. Liquid hydrogen is the apparent inheritor of the role as coldest moderator in high-power systems and yet we don't yet have a body of data describing liquid hydrogen, and we need it if we are going to design good moderators. So one of the important issues that arose in our discussion was the need for a better understanding and a design basis for liquid hydrogen systems (this includes para- and ortho-hydrogen and their mixtures). We need scattering kernels, benchmark calculations and experiments.

> *What's actually needed for these hydrogen kernels to do a good job on thermalisation, is an energy transfer range down to a fraction of an meV and up to several hundreds or thousands of meV (where the kernel becomes independent of the chemical state).*

Gary Russell: Basically, there are three ways of doing neutronic design calculations for complex spallation neutron source systems: a) deterministic transport methods, b) Monte Carlo techniques and c) Walter Fischer's handmade physics. A simplistic view of these different approaches is as follows:

- Deterministic transport methods generally provide "exact solutions" to approximations of the Boltzmann transport equation. Computing errors are systematic, and, aside from uncertainities in the cross section data, arise not only from the discretization of the time-space-angle-energy phase space for numerical computations but also from the fact that, with rare exceptions, full representations of three-dimensional configurations cannot be done. One might paraphrase the deterministic transport approach as potentially giving the right answer to the wrong problem.

- Monte Carlo techniques are used to solve the Boltzmann equation directly. With this method, one can study very complex three-dimensional configurations, and the continuous treatment of energy, space, and angle makes discretization errors in Monte Carlo calculations take the

form of stochastic uncertainties; however, one has to careful that all relevant parts of phase space have been properly sampled and that the problem has converged. In Monte Carlo, two approaches are generally utilized: a) non-analog Monte Carlo, where variance reduction techniques are employed to reduce running time and variance in the problem answer, and b) analog Monte Carlo, which involves a direct computer simulation of physical laws. One may loosely describe the Monte Carlo technique as possibly giving the wrong answer to the right problem.

- Walter Fischer's handmade physics employs one's gut feelings and uses simplified approaches to elicit answers to problems. This strategy is perhaps the most gratifying of all. However, it has been my experience for complex spallation neutron source designs, that intuition can only carry you so far. A good example of this is the LANSCE split-target, flux-trap-moderator target system.

In all cases, the bottom line is that neutronic calculations for complex spallation neutron source design are intricate, and care needs to be taken to assure the answers are believable.

As mentioned above, using the Monte Carlo approach, one can mock-up complex geometries quite well, but the physics must also be right. The physics comes in via the cross sections used; a weak link at low energies is the availability and adequacy of scattering kernels. This is particularly true for liquid hydrogen where more work most certainly is required. Hydrogen is further complicated by the necessity of proper accounting of ortho- and para-hydrogen effects.

The issue of liquid hydrogen scattering kernels came up in the target and moderator session when I was going through some details as to how the LANSCE moderator sizes were chosen. In the LANSCE cold moderator studies, I used a hydrogen kernel gotten from our Jülich collaborators, who, in turn, obtained the kernel from A. Robert of ILL. I cannot comment in detail on the physics of the kernel except for the following general remarks: a) the Young and Koppel formalism for molecular hydrogen gas is used, and b) the kernel should be applicable to liquid hydrogen for neutron energies above 7 meV. This latter restriction is not too comforting, but the severity of the implication depends on how important "liquid effects" are below

7 meV in a practical application. Nevertheless, that is all I had available, and I used it in the LANSCE liquid hydrogen moderator design.

To checkout my calculational procedure for the LANSCE target system, I did a sequence of computations where I varied the thickness of the liquid hydrogen moderator, and another series were I changed the moderator ortho/para composition. My results agreed qualitatively with similar calculations performed by Ralph Neef of Jülich. These latter were done to optimize a liquid hydrogen moderator for the DIDO reactor in Jülich; the same hydrogen kernel was used in both calculations. Since the two computations were done for radically different geometries, the qualitative agreement gave me confidence in my calculational approach. My conclusions were similar to theirs, and we chose the LANSCE hydrogen moderator thickness to be 5 cm. Without regard to neutron pulse width questions, my choice of moderator thickness was based on the following: a) do not sacrifice the integrated (E <10 meV) cold neutron intensity, b) keep energy deposition in the moderator as low as possible, c) more-or-less minimize the effects of differing para-hydrogen concentrations on the integrated cold neutron intensity.

A more stringent test of the adequacy of the hydrogen kernel comes about when comparing measured neutron leakage spectra from a moderator with calculated predictions. Spectra from liquid hydrogen moderators have been measured at ISIS and LANSCE. The ISIS result was obtained during a commissioning run in December of 1984. Phil Seeger recently measured a spectrum at LANSCE, and showed the results at this meeting. A common characteristic of these two spectra is a conspicuous "bump" showing a rise in the neutron intensity in the 10-20 meV energy range. This effect is generally attributed to the rise in the para-hydrogen cross section which also occurs in that general energy realm. In the target and moderator session, Andrew Taylor noted that at the RAL they were unsuccessful in calculating the details of the observed spectrum, and knew of no scattering kernel which reproduced the observed "bump". It was a general consensus that the state-of-affairs of kernels for liquid hydrogen was precarious.

Last evening, I did an "eyeball" comparison between my preliminary calculation of the neutron spectrum leaking from the LANSCE liquid hydrogen moderator and Phil Seeger's measurement. I get agreement of order 25% for integrals of the data from 10-50 meV and below 10 meV. I also plotted

my calculated spectrum on the figure Günter Bauer showed when reporting ISIS moderator performance. My calculated spectrum differs significantly from the spectrum in Günter's figure, and qualitatively has features similar to the ISIS measurement. We must and will be more definitive in these comparisons, and should also concern ourselves with the effects of ortho and para concentrations on neutron pulse widths.

Liquid hydrogen moderators could prove to be very important in high-power spallation neutron source applications. We need reliable "tools" to design these moderators. I would ask those individuals who are working on an improved kernel formalism or those who are contemplating doing so to forge ahead. We need these new tools and better benchmark measurements (with which to compare) if we are to push spallation neutron source performance to the limit.