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COMPARISONS OF MCNP THERMAL SCATTERING KERNELS IN A CALCULATION OF THE SPECTRUM FROM THE RAL LIQUID HYDROGEN MODERATOR.

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ABSTRACT

A comparison was made between MCNP calculations, for varying ortho/para concentrations, with experimental measurements of the neutron spectrum from the ISIS liquid hydrogen moderator.

The original calculations were performed using the standard $S(\alpha, \beta)$ thermal scattering kernels, HPARA and HORTHO. Unfortunately the agreement between the calculated and measured spectra was poor. In particular, the calculated flux showed strong fluctuations with energy, which are not seen in the measured spectra.

This problem was reported by other authors, including G. Russel et al., during the Cold Moderator workshop at Argonne, Sept. 28 - Oct 2 1997. It was reported that the cause had been identified; the angular bin structure used in the preparation of the kernels was too coarse. A new set of kernels (PARAH and ORTHOH) had been calculated using finer bins, and had been shown to produce reasonable results. It was agreed that these kernels would be made available to workshop participants on a pre-release basis.

We subsequently repeated our calculations with the new kernels, and our results also show greatly improved agreement between measured and calculated spectra. A best fit was obtained for 100% para hydrogen, and the new results showed close agreement between calculated and measured spectra up to about 5.5 Å. For longer wavelengths the results diverge, with the calculated fluxes apparently overestimating the measured spectrum.

Keywords: Kernels, ISIS, hydrogen, moderator

1. Introduction

An original set of calculations on the ISIS liquid hydrogen moderator was presented at the Cold Moderator Workshop, for varying ortho/para compositions 1. For these calculations we applied a patch to MCNP to permit the mixing of $S(\alpha, \beta)$ scattering laws for ortho- and para-hydrogen. Unfortunately a bug was found in the modified code; it apparently failed [2] to calculate a correct value for the total cross section of an ortho-para mixture.

We therefore repeated all our calculations using a well-tested scheme [3] involving modified copies of cross section sets. For para-hydrogen we used the standard neutron scattering and thermal $S(\alpha, \beta)$ cross sections, but for ortho-hydrogen we prepared copies with a fictitious atomic mass number (but with the actual atomic mass left unchanged.) Para-hydrogen and ortho-hydrogen then had separate nuclide identifiers and could be mixed without any modifications to MCNP itself.

Section 2 summarizes the results of our comparison between measured and calculated spectra from the liquid hydrogen moderator at RAL. The results from the original kernels show poor agreement between measurements and calculations. The calculated spectra show spurious structure which is not seen in the measurements. This problem had been seen by others at the Workshop, and its cause had been diagnosed as a deficiency in the preparation of the standard MCNP kernels [5]. We have now repeated our calculations using corrected kernels [4] which were made available to Workshop participants. The results show a dramatic improvement in the agreement between calculated and measured data, although the fit is still not perfect.

Our conclusions, and suggestions for future studies, are given in Section 3.

2. Comparisons between calculated and measured spectra from the RAL liquid hydrogen moderator.

The calculations were carried out using the LCS codes (LAHET and HMCNP4A). A series of HMCNP4A cases was run to determine the variation in the neutron spectrum with ortho-hydrogen concentration.

All the results presented in this section have been repeated using the reliable method described in Section 1, in which ortho/para mixing is achieved using modified cross section files. Two other improvements were made: a finer energy bin structure was specified, and the spectrum was corrected for transmission through aluminium.

Fig. 1 shows the geometry of the aluminium transmission calculation. A uniformly distributed and outwardly directed source was specified at the moderator surface. The angular dependence of the source was chosen so that the flux close to the moderator surface obeyed a cosine distribution ($\phi(\theta) \propto \cos\theta$ where θ is the angle relative to the normal.) The spectrum used for the source was the calculated spectrum for pure para-hydrogen. A temperature of 20K was specified for the liquid hydrogen and the innermost can. Other materials were at ambient temperature (300K).

A special 'scoring region' was defined at a distance of 15cm from the moderator surface, and the flux in the scoring region was calculated. The aluminium cans of the hydrogen moderator were then

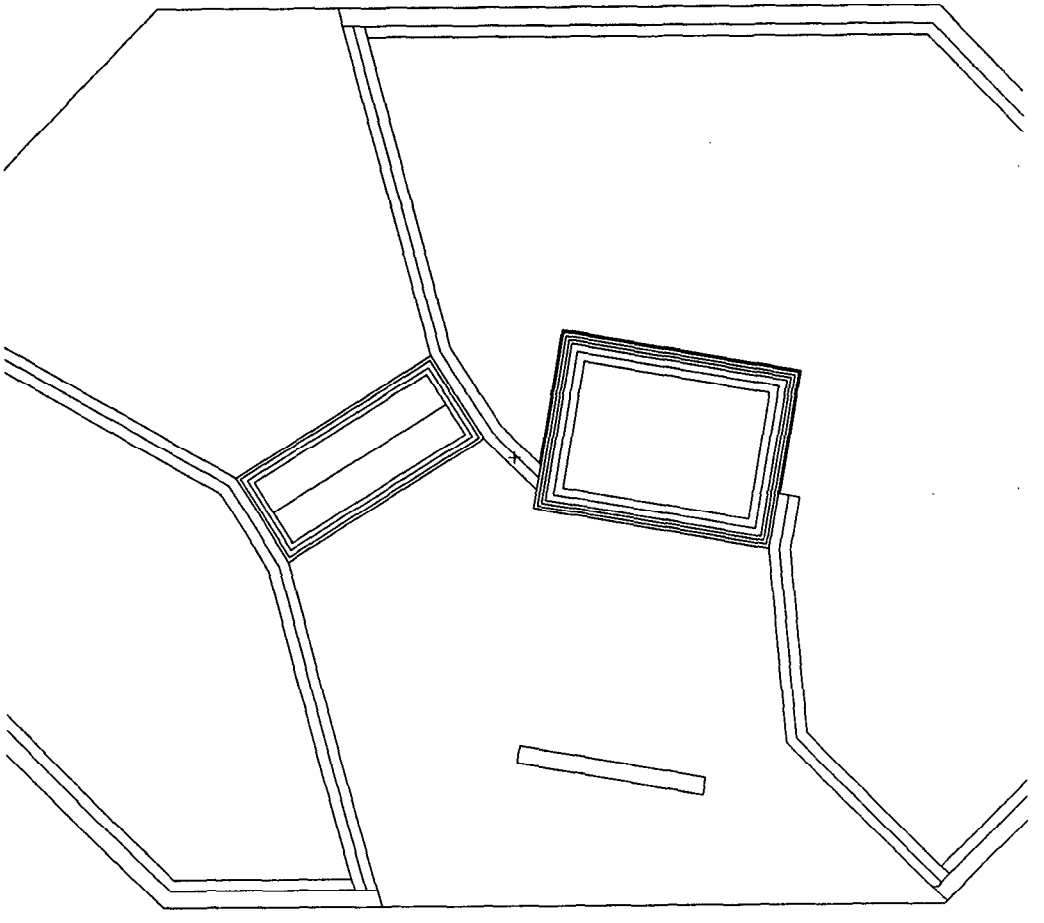

Fig. 1. Geometry used for the aluminium transmission correction, showing the liquid hydrogen moderator (right) and its three aluminium cans, and the 'scoring region' (below).

replaced by void cells, and the calculation repeated. The ratio between the two sets of results was used as a correction factor.

The accuracy of our correction factor is limited by the lack of a suitable scattering kernel for aluminium; the free gas model had to be used and therefore the results do not take into account the long-wavelength effects, e.g. Bragg scattering, which are clearly evident in the measured spectrum. The calculated factor did not vary greatly with wavelength in the range of interest (up to about 7Å) and therefore had little effect on the shape of the calculated spectrum.

Results which used the standard HPARA and HORTHO scattering kernels were unsatisfactory because the calculated spectra exhibited spurious structure which is not present in the measured spectrum (see Figs. 2 and 3). The presentation of G.Russel et al. [5] confirmed this finding. They had diagnosed the cause as the use of insufficiently fine angular bins in the preparation of the data. The kernels had been recalculated and it was shown that the resulting spectra agreed much more closely with experimental measurements. Although the new kernels [4] (PARAH and ORTHOH) will not be released to the general user community until later in 1988, it was announced that they would be made available to Workshop participants. We subsequently obtained the new kernels and used them in a new set of calculations.

Figs. 2 and 3 compare the calculated spectra for low ortho-H_2 concentrations with the measured spectrum. Fig. 2 shows the results calculated using the standard ORTHOH/PARAH kernels, and Fig. 3 shows the results with the improved HORTHO/HPARA kernels. In each case the measured spectrum is shown, normalized to give the best fit to the 100% para-H_2 case. For completeness the corresponding results for higher ortho-H_2 concentrations are also shown, in Figs. 4 and 5.

3. Conclusions

The results, particularly when calculated with the new kernels, uphold our earlier conclusion that the best fit to the measured spectrum occurs for pure para-hydrogen.

It is clear that the new kernels provide the expected improvement in the calculated results, which are now much closer to the experimental measurements. Up to about 5.5Å the agreement between the calculated curve for 100% para-hydrogen with the measured curve (Fig. 3) is within about 10%. However, the curves appear to diverge at longer wavelengths. In order to clarify this issue, it would be desirable for the experimental measurements to be extended to longer wavelengths and for a more accurate estimate of the aluminium transmission factor to be used.

Another issue for future study is the approximate geometry used in the current ISIS model, in which a rectangular form is used for all moderators (see Fig. 1). It would be desirable to determine whether a more realistic moderator geometry, using curved surfaces with appropriate radii, would further improve the agreement between the calculated and measured spectra.

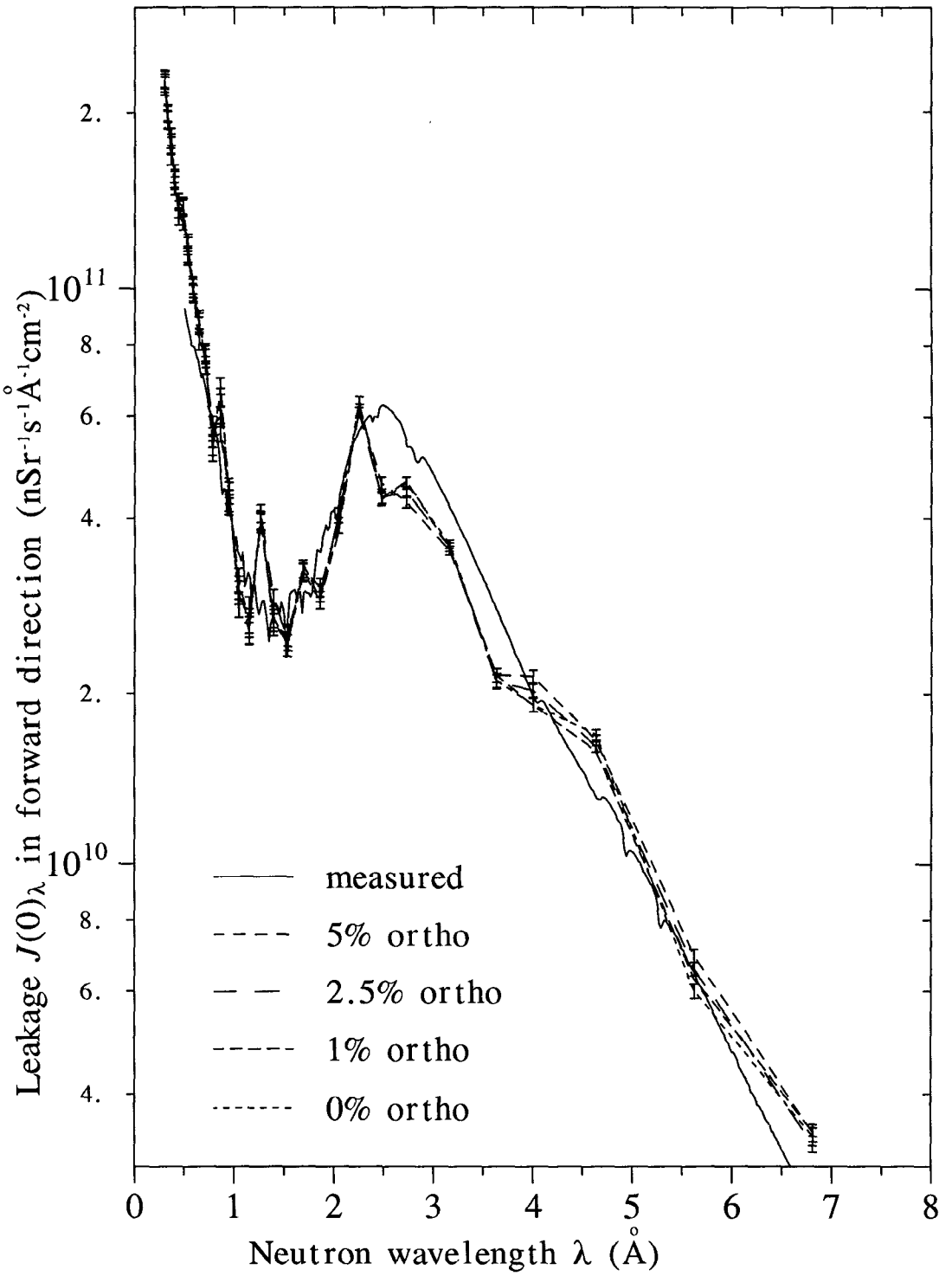

Fig. 2. Comparison of experimentally measured with calculated spectra for low ortho-H_2 concentrations using the standard (PARAH/ORTHOH) kernels.

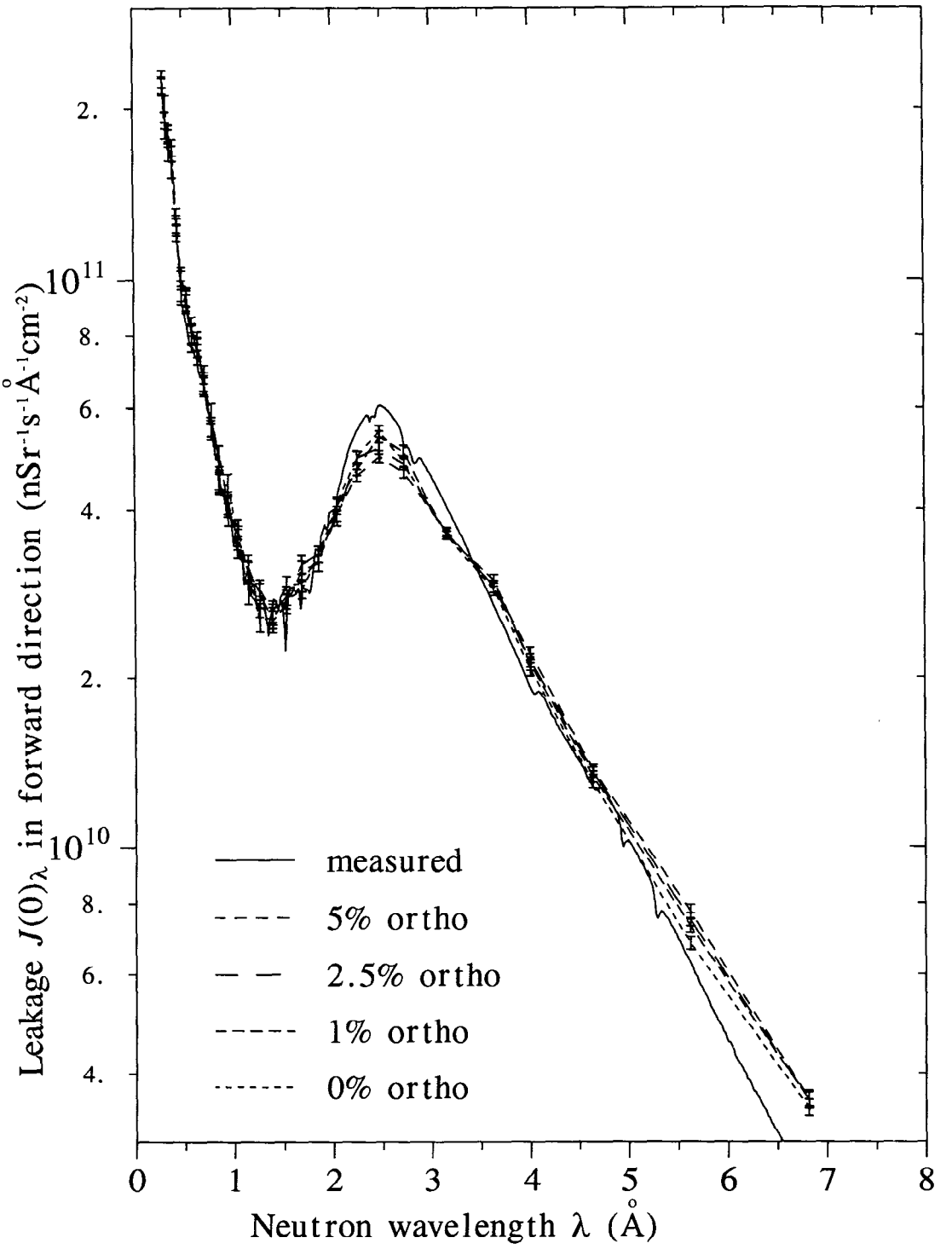

Fig. 3. Comparison of experimentally measured with calculated spectra for low ortho-H_2 concentrations using the new (HORTHO/HPARA) kernels.

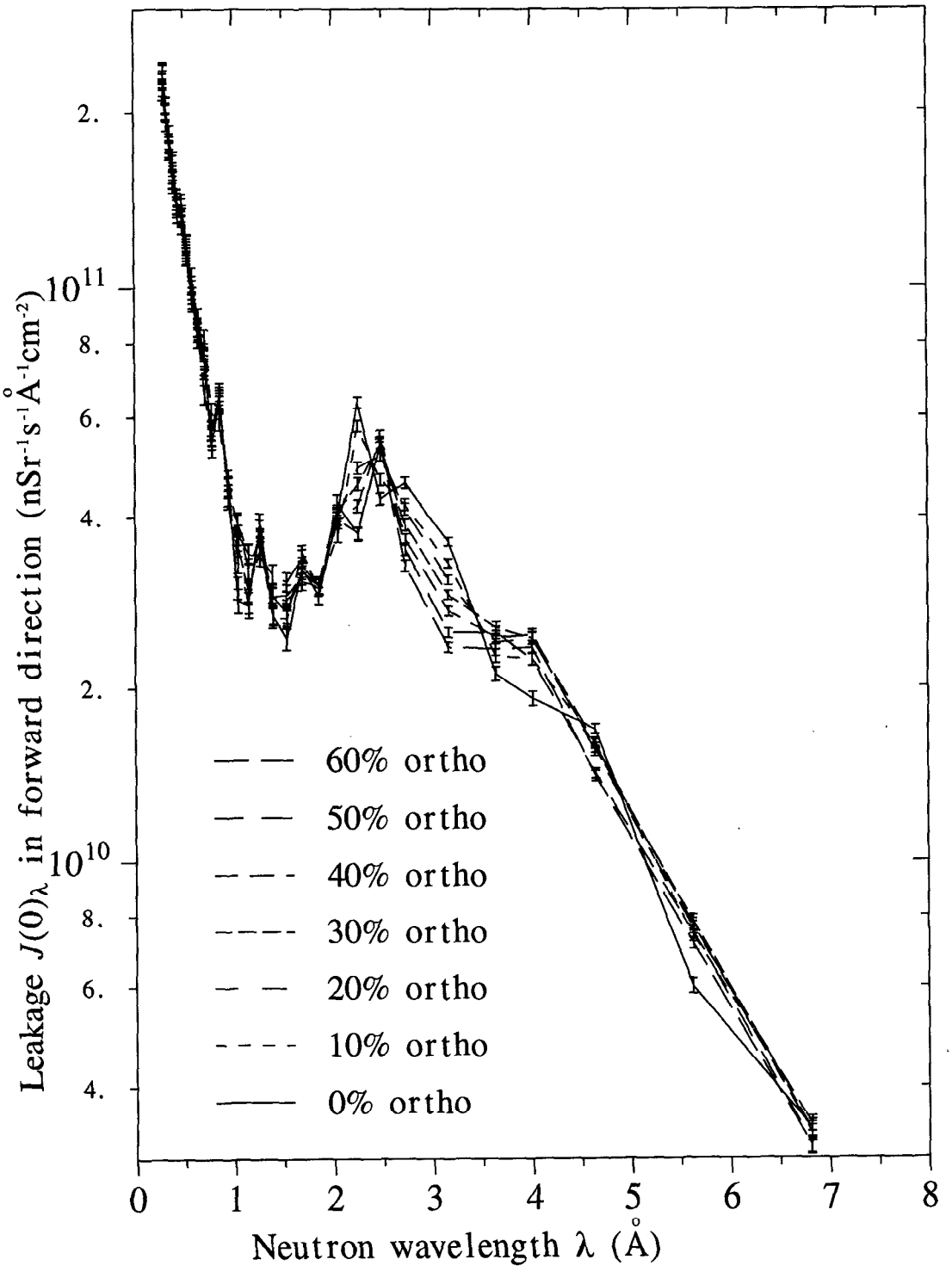

Fig. 4. Calculated spectra for high ortho-H_2 concentrations with standard PARAH/ORTHOH kernels.

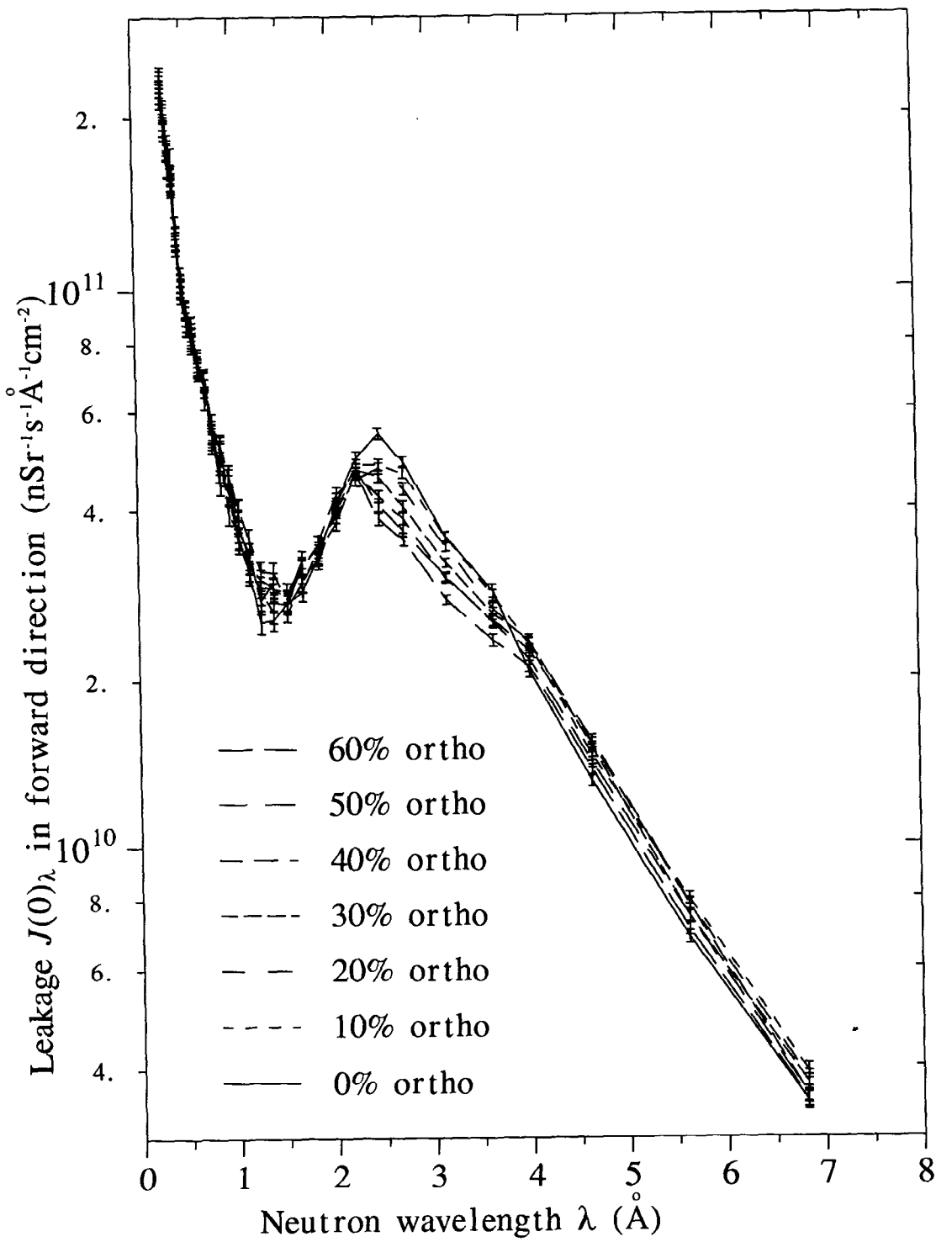

Fig. 5. Calculated spectra for high ortho-H_2 concentrations with the new (HORTHO/HPARA) kernels. correction.

4. References.

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