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MODIFICATIONS TO THE FLANGE CODE FOR WATER SCATTERING KERNELS

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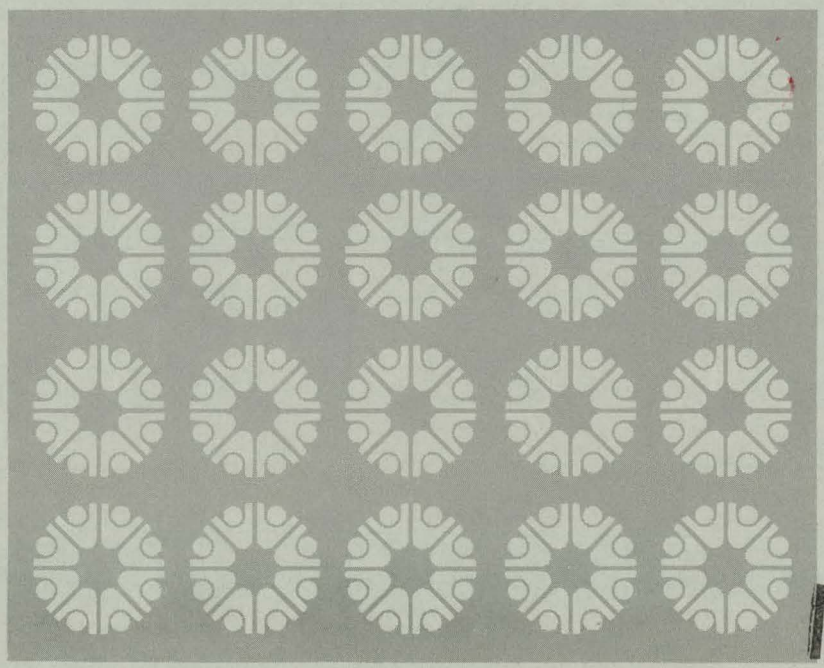

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MODIFICATIONS TO THE FLANGE CODE FOR WATER SCATTERING KERNELS

by

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INTRODUCTION AND SUMMARY

The FLANGE[1] code is the code approved to process ENDF/B[2] thermal neutron scattering data. It was found that the integration scheme used to calculate the scattering cross sections for hydrogen in water gives errors of up to 1-1/2 percent in the total scattering cross section and up to 3-1/2 percent in the transport cross section for energies above 0.6 eV. The scattering cross section also has a scatter of approximately one percent for different energies. Improvements to the integration were made which reduced the systematic error and scatter in the cross section to less than 0.2 percent. Changes were also made in the code which speed up the calculation by as much as a factor of three yet give values identical to those of the slower calculation.

The FLANGE code was used with ENDF/B data to produce a scattering kernel for hydrogen in water for the BMC Monte Carlo code.[3] This kernel consistently gave a harder spectrum than calculations using the THERMOS code with a kernel also calculated using the FLANGE code with the same data. It has been determined that this discrepancy is explained by the integration scheme used in the FLANGE code. A new kernel for the BMC code has been generated using the improved version of the FLANGE code.

The modified FLANGE code is designed to give good cross sections for hydrogen in water. If other moderators are being calculated, an examination of the FLANGE integration scheme should probably be made for that particular moderator.

Inadequacies in the FLANGE Code

The FLANGE code is used to compute thermal scattering cross sections and kernels for codes such as THERMOS.[4] A 60 energy group kernel for hydrogen in water was prepared for the THERMOS code using FLANGE. Examination of the results showed a dip of 1 percent in the scattering cross section at the energy of the ^{240}Pu resonance. The values above 0.6 eV are shown in Figure 1. Notice the scatter in the points as a function of energy. The cause of this was traced to two assumptions being made in the final integration of the scattering cross section over energy in the FLANGE code. First the integration points become farther apart at low energies as the initial energies become higher. Second, the line shape between points is assumed to be linear in the variables log $\sigma(E_0 \rightarrow E)$ versus E_0. Between the lowest energy point and zero energy, it is assumed that the line shape is linear in cross section and energy.

The reason the energy points become farther apart is that the energy points for the cross section integration in FLANGE are picked to correspond to the beta values of the $S(\alpha,\beta)$ data on the ENDF/B data tape and the distance between beta values becomes larger as beta is increased. This produces an accurate integration near the initial energy but the points become too far apart at low energies. The opposite effect is produced if the energy points used for a typical THERMOS kernel are used to integrate the scattering cross section as there are usually quite a few points at low energies but the distance between points becomes larger at higher energies. Hence, a very accurate integral of the scattering to low

energies can be made but the integral near the initial energy may be very poor. The usual procedure used in FLANGE is to integrate the cross section separately and then force the integral of the kernel to agree by varying the kernal value at the initial energy.

The fact that the FLANGE integral should be more accurate for higher energies and the kernel integral more accurate at low energies was used to provide checkpoint. A kernel integral was used up to 0.4 eV and FLANGE was used below 0.4 eV. The resulting check point is included on Figure 1. Note that the check point is about 1/2 percent above where an upper envelope of the unmodified FLANGE points would pass.

If the correct line shape between integration points is assumed, then it does not matter how far the integration points are apart. This leaves the line shape used by FLANGE at low energies suspect. The line shape assumed by FLANGE is compared to the correct shape shown by the points calculated for a kernel in Figure 2. This shows the worst two cases, where the β value from the library gives an energy point just above or just below zero. Note how poorly both a linear line and a line that is linear in log $\sigma(E_0 \rightarrow E)$ versus energy fits the curve at low energies.

It was suggested by Dr. J. L. Carter, Jr. that a line function assuming that $\sigma(E_0 \rightarrow E)$ was linear as a function of $\sqrt{E}$ would give a closer fit for low energies as that is the limiting line function for an ideal gas at low energies. The curve resulting from this line shape is also shown in Figure 2.

Modified Integration Scheme

The integration scheme in FLANGE was modified by using the $\sigma(E_0 \rightarrow E)$ versus $\sqrt{E}$ line shape at low energies and also including up to two extra points for each beta range. The resulting cross sections calculated using these modifications are also shown in Figure 1. It can be seen that the scatter has been greatly reduced and the values agree much better with the result obtained using a combination of FLANGE and kernel integrals. This modified integration scheme takes very little more computer time than the original.

Calculational Speed Reduction

The FLANGE code calculates the differential cross sections $\sigma(E_0 \rightarrow E)$ by integrating $S(\alpha,\beta)$ over alpha for the beta which would result in the energy change $E_0 \rightarrow E$. The α integration is done between the limits α_- and α_+ where

$$\alpha_{\pm} = \frac{E + E_0 - 2\sqrt{EE_0}}{AkT}$$

The integration over α is made using $S(\alpha,\beta)$ values obtained by extrapolating between the β points in the ENDF/B data. Many of these extrapolations are needless and repeated as most of the β values used in the cross section calculations in FLANGE are values which correspond exactly with the β values in the END/B data.

Also, the $S(\alpha,\beta)$ integral over α can be done from the minimum to the maximum value of α and then when $\alpha_{\pm}$ is given the integral can be obtained by integrating only the panels containing α_- and α_+ and subtracting the integral just above the α_- panel from the integral just below the α_+ panel.

When the FLANGE code was modified using the above observations, it was found that the time needed to calculate a 60 group kernel dropped from 602 seconds to 198 seconds, resulting in a factor of three increase in calculational speed. It should be noted that these changes are not based on introducing approximations but give answers identical to those of the slower calculation.

Differences Between the BMC and THERMOS Kernels

It has been determined that these modifications result in a much better agreement in comparative calculations using the BMC Monte Carlo and the THERMOS kernels. The BMC kernel was designed to reproduce the FLANGE line shape which resulted in too little scatter into the low energies. The modified FLANGE code uses a more nearly correct line shape which should improve the BMC kernel. The THERMOS kernel gave the correct amount of scattering into the low energy groups but not enough scattering into the initial energy group. The modified FLANGE code calculates the cross section more accurately so the THERMOS kernel should also be more accurate. The net effect of using the modified FLANGE code to calculate the two kernels has been to slightly harden the THERMOS calculated spectrum while slightly softening the BMC calculated flux spectrum. They now will agree much better.

The Effect on the Transport Cross Section

The calculation of the first moment cross section was also modified slightly. A linear representation of the line function was used for down scattering. This resulted in a very slight change in the integrated first moment cross section. Hence the transport cross section is changed due to the change in the scattering cross section. The transport cross

section can have a change of up to 3 percent due to a 1-1/2 percent change in the scattering cross section. This much change may result in a difference in some calculations using codes such as THERMOS.

CONCLUSIONS

It can be argued that the approximately 1 percent increase in the cross sections using the modified FLANGE is not important as this is within the accuracy of the cross section data; however, it seems best not to introduce needless uncertainties due to inadequate numerical integrations of cross sections to the other necessary approximations in reactor physics calculations. With these few modifications to the FLANGE code, the calculational accuracy is increased to a point where the numerical uncertainties in the kernel are not a problem. Also, the cost of calculating new kernels is greatly reduced.

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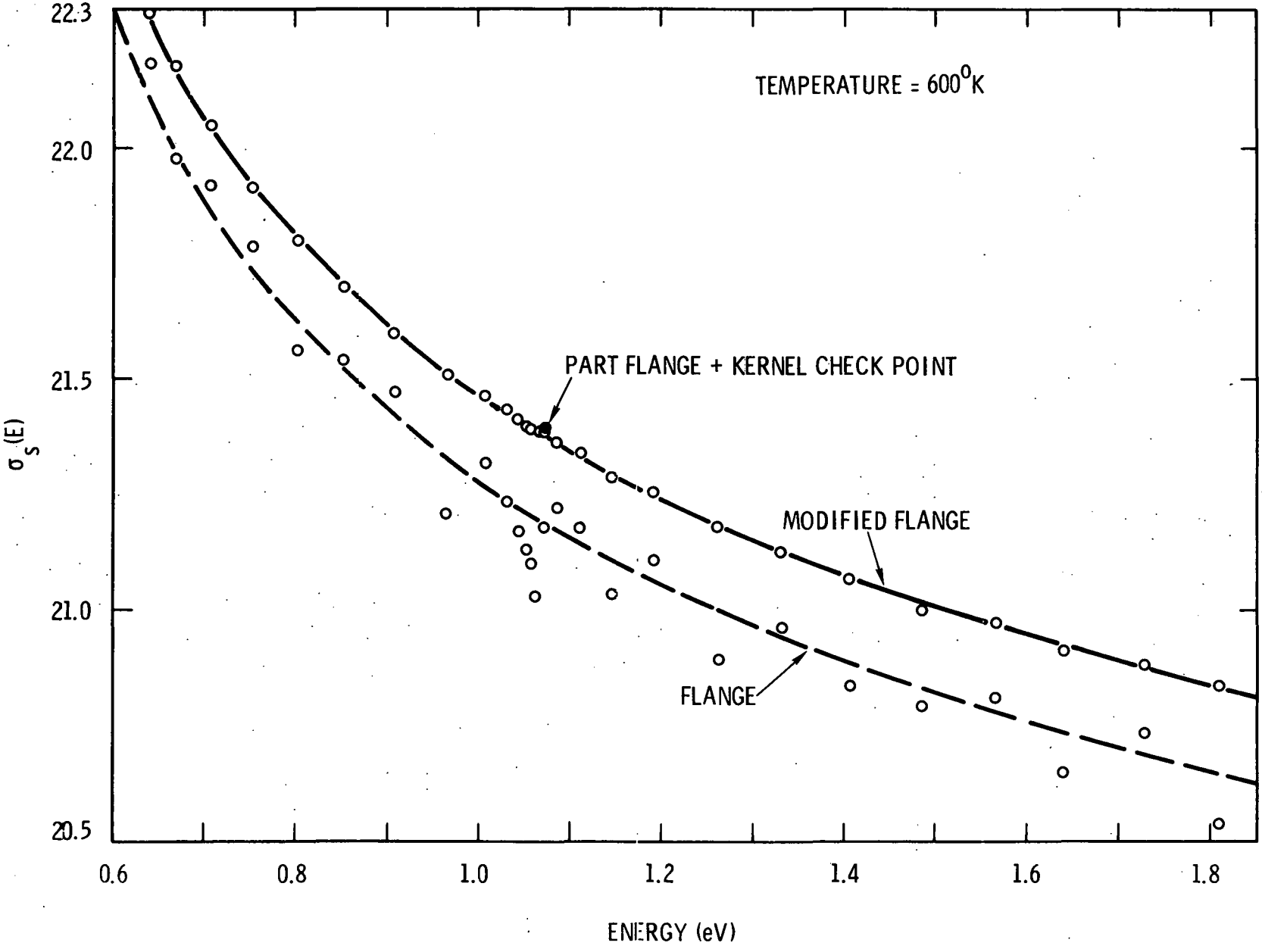

FIGURE 1 - $\sigma_s(E)$ VERUS E - HYDROGEN IN WATER CALCULATED USING FLANGE

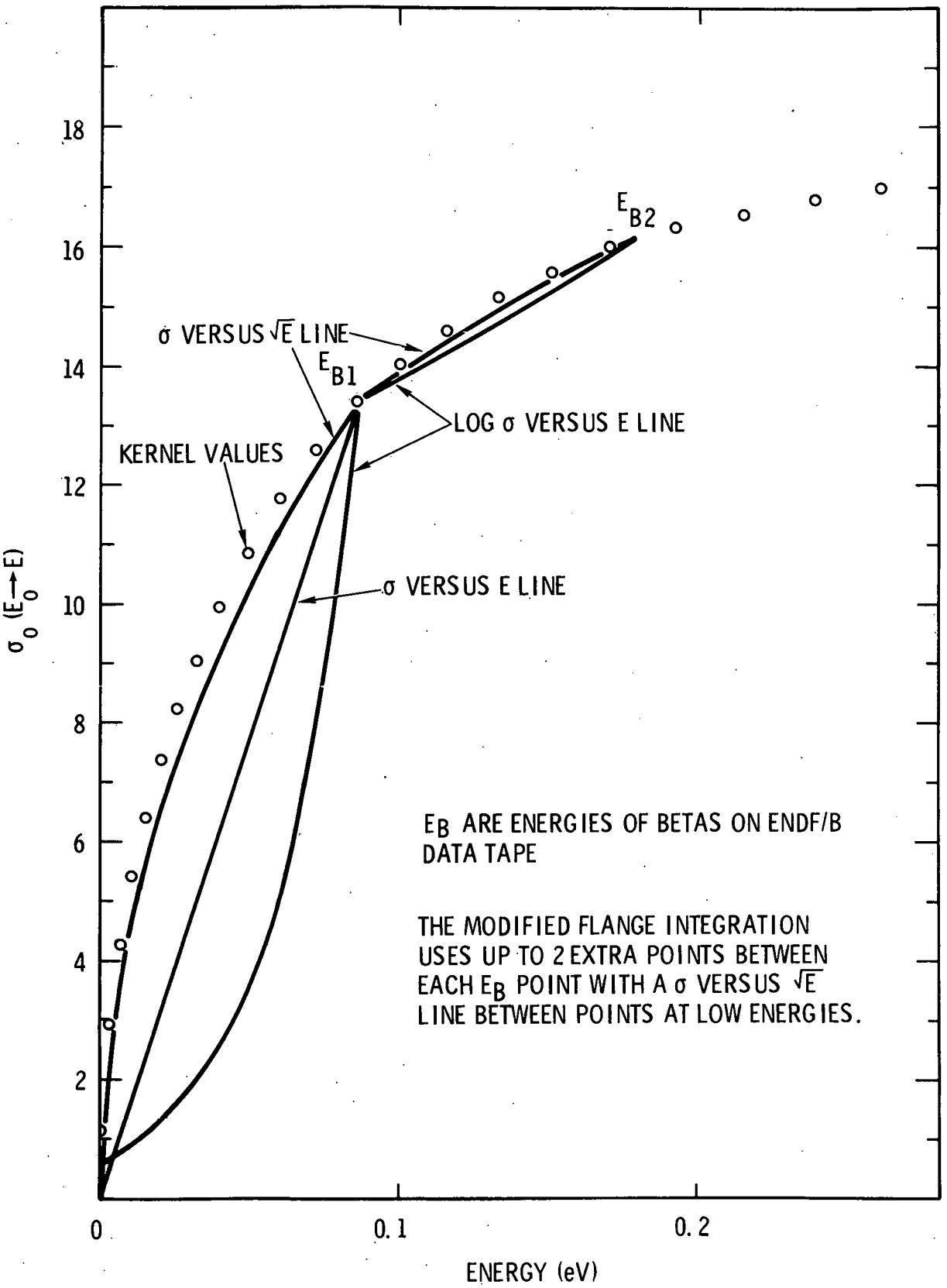

FIGURE 2 - PLOT OF σ $(E_0 \rightarrow E)$ VERSUS E FOR E_0 = 1.145 eV. SHOWING HOW VARIOUS LINE SHAPES FIT THE DATA AT LOW ENERGIES.

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