INTRODUCTION

In the modeling and analysis of neutron transport, the neutron interaction probability with a target material must be properly accounted for. These interaction probabilities, or cross sections, are strong functions of the target material temperature and the incident neutron energy. In neutron transport codes, it is typical to store cross sections at many temperatures and energies based on the transport problem being modeled. For coupled neutron-thermal-hydraulic problems, pre-storing cross section data becomes memory intensive because of the fine temperature mesh required to account for temperature feedback. In recent years, data storage has been significantly reduced in the resolved-resonance and epithermal energy regions with on-the-fly strategies. These methods assume a Maxwell-Boltzmann distribution in the target nuclide energy, making it possible to derive the analytical temperature dependence of the cross sections. At thermal neutron energies, however, this assumption is not valid due to the dominance of chemical binding effects.

This work focuses on a new strategy to treat the temperature dependence of double differential scattering data in the thermal energy region by examining the temperature dependence of cumulative distribution functions (CDFs) in the parameters that define the thermal scattering law, \( S(\alpha, \beta) \). A method proposed by Ballinger [1] is introduced to construct probability density functions (PDFs) of momentum transfer (\( \alpha \)) and energy transfer (\( \beta \)). The CDFs of these PDFs are then constructed on a temperature mesh and an incoming energy mesh for common moderator nuclei. Regression models are then used to fit the temperature dependence of these CDFs. The best functional fits are chosen based on an error analysis procedure and the outgoing parameters are then sampled on-the-fly from the coefficients of the chosen functional fits.

This paper is based on previous work published earlier in the year [2], but with modifications to the fineness of the meshes used. The results presented in this paper use these new results.

MOTIVATION

The incoherent inelastic differential scattering cross section in the thermal region is classically denoted by

\[
\sigma(E \rightarrow E', \Omega \cdot \Omega', T) = \frac{\sigma_b}{2kT} \int \frac{E}{E'} e^{-\beta} S(\alpha, \beta, T),
\]

where \( E \) and \( E' \) represent the pre- and post-collision energy, respectively, \( \Omega \cdot \Omega' \) is the scattering angle, \( \sigma_b \) is the bound atom cross section, \( kT \) is the ambient temperature and \( S(\alpha, \beta, T) \) is the scattering law which contains the quantum translational, rotational, and vibrational motions of the neutron. The quantities \( \alpha \) and \( \beta \) represent, respectively, momentum and energy transfer,

\[
\alpha = \frac{E + E' - 2\mu \sqrt{EE'}}{A_0 kT},
\]

\[
\beta = \frac{E - E'}{kT},
\]

where \( A_0 \) is the target nucleus to neutron mass ratio and \( \mu \) is the cosine of the scattering angle. Scattering law data are generated with the nuclear data processing code NJOY [3] and stored in ENDF thermal scattering files [4] for select moderator materials at specific temperatures and on an \((\alpha, \beta)\) mesh. Modern Monte Carlo codes (MC21 and MCNP6 [5]) use a continuous-in-energy representation for the outgoing scattering parameters, requiring a very fine energy mesh. Even for a single temperature, the \( S(\alpha, \beta, T) \) data can be large as shown in Table I for selected moderators at room temperature from the ENDF/B-VII.1 library.

Because many temperature sets are often needed, the memory load needed can become unnecessarily large. The approach we take is based on CDFs of \( \alpha \) and \( \beta \) from the \( S(\alpha, \beta, T) \) data. If a temperature-dependent functional form can be provided for the thermal scattering data, the data storage can be substantially decreased. In this paper, we examine the temperature dependences of the CDFs in \( \alpha \) and \( \beta \) for the isotopes graphite and hydrogen bound in light water. Functional forms with different regression models are studied to fit the examined temperature dependences. The fitting coefficients with minimum fitting errors are identified to eliminate the need to store continuous \( S(\alpha, \beta, T) \) datasets at all temperatures. These fitting coefficients could then be used in the future to sample \( \alpha \) and \( \beta \) (and thus scattered energy and scattering angle) at any temperature on-the-fly in Monte Carlo simulations.

\[
\text{Table I. Percent error as a function of distance.}
\]

<table>
<thead>
<tr>
<th>Distance (cm)</th>
<th>Percent Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>175</td>
</tr>
<tr>
<td>10</td>
<td>90</td>
</tr>
<tr>
<td>20</td>
<td>50</td>
</tr>
<tr>
<td>50</td>
<td>35.5</td>
</tr>
<tr>
<td>70</td>
<td>7.7</td>
</tr>
<tr>
<td>90</td>
<td>6.3</td>
</tr>
</tbody>
</table>

\[
\text{The theoretical values are:}
\]

\[
\gamma/n \text{ Ratio, Measured: 0.1, 0.5, 2.0, 5.0, 10.0, 20.0, 50.0, 100.0, 200.0, 500.0.}
\]

\[
\text{The experimental values are:}
\]

\[
\gamma/n \text{ Ratio, Measured: 0.1, 0.5, 2.0, 5.0, 10.0, 20.0, 50.0, 100.0, 200.0, 500.0.}
\]
Table I. ENDF/B-VII.1 Continuous \( S(\alpha, \beta, T) \) file sizes for selected moderator materials at room temperature

<table>
<thead>
<tr>
<th>Material</th>
<th>File Size [MB]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphite</td>
<td>24</td>
</tr>
<tr>
<td>Water</td>
<td>24.9</td>
</tr>
<tr>
<td>U in UO₂</td>
<td>50</td>
</tr>
<tr>
<td>O₂ in UO₂</td>
<td>75</td>
</tr>
<tr>
<td>Zr in ZrH</td>
<td>56</td>
</tr>
<tr>
<td>H in ZrH</td>
<td>116</td>
</tr>
</tbody>
</table>

METHODOLOGY

The sampling procedure described here is based on the direct sampling method used by Ballinger [1]. The sampling is performed on the PDFs of the energy and momentum transfer,

\[
p(\beta | E, T) = \frac{e^{-\beta/2} \int_{\alpha_{\min}}^{\alpha_{\max}} S(\alpha, \beta, T) d\alpha}{\int_{\beta_{\min}}^{\beta_{\max}} \int_{\alpha_{\min}}^{\alpha_{\max}} e^{-\beta/2} S(\alpha, \beta, T) d\alpha d\beta}, \quad (4)
\]

\[
p(\alpha | \beta, E, T) = \frac{S(\alpha, \beta, T)}{\int_{\alpha_{\min}}^{\alpha_{\max}} S(\alpha, \beta, T) d\alpha}. \quad (5)
\]

Assuming a given initial energy \( E \) at some temperature \( T \), a value of beta can be sampled from Eq. (4). Then, once this is done, Eq. (5) is used to sample a value of alpha. From these sampled values, the scattered energy and cosine of the scattering angle can be directly calculated. Fig. 1 shows an example of the beta CDF generated for graphite at an incoming energy of 1 eV at five temperatures.

The temperature dependence of the \( \beta \) CDF was examined at discrete CDF probability lines in the range \([0.025, 0.975]\) (39 probability lines per energy) and on a mesh of incoming neutron energies in the range \([1E-5, 3.75]\) eV (106 total energies) for graphite. In total, there were four variables considered in the analysis: \( E_{\text{in}}, \beta, T \) and \( P_{\beta} \), where \( P_{\beta} \) is the \( \beta \) CDF probability. The \( \alpha \) CDF temperature analysis consists of the four variables: \( \beta, \alpha, T \) and \( P_{\alpha} \), where \( P_{\alpha} \) is the \( \alpha \) CDF probability. Although the \( \alpha \) PDF/CDF is also dependent on the incoming neutron energy, this variable is ignored to reduce the data storage. Instead, the CDF is analyzed over the entire given \( \alpha \) mesh instead of between \( \alpha_{\min} \) and \( \alpha_{\max} \). Then, the \( \alpha \) bounds are calculated as needed for the desired incoming neutron energy and the appropriate section of the \( \alpha \) is sampled. Note that the \( \beta \) mesh for graphite consists of 96 values in the range \([0, 80]\).

Functional expansions based on different regression models are examined to fit the \( \beta(T) \) and \( \alpha(T) \) data at different values of alpha and beta CDFs. This temperature dependence was performed on a mesh of 35 values in the range \([300, 2000]\) K at 50 K increments for graphite. A code was developed to build the CDFs for beta and alpha at each temperature in the mesh from \( S(\alpha, \beta, T) \) data obtained from NJOY. The \( \beta(T) \) data are then outputted at each beta and \( P_{\beta} \) in their respective meshes. Likewise, the \( \alpha(T) \) data are outputted at each beta and \( P_{\alpha} \) in their respective meshes. A visualization of this procedure is given in Fig. 2 for the beta data. In the figure, only five temperatures (300K, 650K, 1000K, 1500K and 2000K) are shown along with four probability lines (0.2, 0.4, 0.6 and 0.8) for one incoming energy value (1 eV). This is for visualization only. In actuality, the meshes used are finer.

Along each CDF probability line, the temperature dependence is examined through fitting functions. The next section compares different temperature fitting functions to the alpha and beta CDFs for graphite.

RESULTS

To determine the best fit for the data, eight different regression models were considered, shown in Table II. The \( a_i \)'s are the fitting coefficients and \( N \) is the order of the functional expansion. To determine the best fit for \( \beta(T) \) and \( \alpha(T) \), a general least squares method is used and the root-mean-square error (RMSE) is calculated at every CDF probability, incoming energy, and beta value. The RMSE is given by

\[
RMSE = \sqrt{\frac{N_T \sum_{i=1}^{N_T} (\theta_i - \theta_{i,\text{fit}})^2}{N_T - (N + 1)}}, \quad (6)
\]
order is best to use, the change in the average RMSE between adjacent expansion orders for a fit should be small. It was decided to choose Fit 4 with $N=2$ for the $\beta(T)$ data and Fit 2 with $N=4$ for the $\alpha(T)$ data. The total storage size of these coefficients is roughly 461 kB and can be used to sample secondary parameters for any temperature and any energy. This is a substantial improvement from the original 24 MB storage per temperature.

Table III. Average RMSE for $\beta(T)$ for graphite.

<table>
<thead>
<tr>
<th>Fit</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>N=1</td>
<td>0.1198</td>
<td>0.0208</td>
<td>0.0934</td>
<td>0.0421</td>
</tr>
<tr>
<td>N=2</td>
<td>0.0552</td>
<td>0.0059</td>
<td>0.0329</td>
<td>0.0051</td>
</tr>
<tr>
<td>N=3</td>
<td>0.0269</td>
<td>0.0031</td>
<td>0.0119</td>
<td>0.0030</td>
</tr>
<tr>
<td>N=4</td>
<td>0.0135</td>
<td>0.0024</td>
<td>0.0048</td>
<td>0.0023</td>
</tr>
</tbody>
</table>

Table IV. Average RMSE for $\alpha(T)$ for graphite.

<table>
<thead>
<tr>
<th>Fit</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>N=1</td>
<td>0.1866</td>
<td>0.0480</td>
<td>0.1571</td>
<td>0.0844</td>
</tr>
<tr>
<td>N=2</td>
<td>0.0986</td>
<td>0.0234</td>
<td>0.0637</td>
<td>0.0289</td>
</tr>
<tr>
<td>N=3</td>
<td>0.0527</td>
<td>0.0175</td>
<td>0.0289</td>
<td>0.0174</td>
</tr>
<tr>
<td>N=4</td>
<td>0.0295</td>
<td>0.0142</td>
<td>0.0174</td>
<td>0.0149</td>
</tr>
</tbody>
</table>

To test the goodness of these coefficients, a simple Monte Carlo code was written to sample alpha and beta many times using only the coefficient files. Linear interpolation is performed to intermediate values in the energy and beta meshes when necessary. A plot of the energy (or beta) mesh versus the relative frequency of each sampled beta (or sampled alpha) reproduces the beta (or alpha) PDF. Integrating over this produces the CDF. This is then compared to the true CDF found from the true $S(\alpha, \beta, T)$ data at the incoming energy, beta value and temperature. Figs. 3 and 4 show the relative errors between the true values and the estimated values found from the fitting coefficients for the beta CDF and alpha CDF, respectively.

From Figs. 3 and 4, the largest relative errors occur for high CDF probability values. This is because the standard deviation for the number of sampled values that fall inside the bins with CDF values greater than 0.975 is large, resulting in large errors. To remedy this, more samples could be run to obtain more values in these bins, lowering the standard deviation. However, for the majority of the CDF region, the relative error is small.

**FUTURE TESTING IN MCNP6**

A general least squares fitting method was used to determine the best functional fit to the alpha and beta CDF data. Random sampling of alpha and beta using the coefficient files was compared to sampling alpha and beta from the actual $S(\alpha, \beta)$ datasets. Although the relative differences between the two methods were small, these
differences have not been applied to the calculation of reaction rates, k-eigenvalue, etc. in the thermal range. It is intended to soon modify the MCNP6 source code to allow thermal neutron incoherent inelastic scattering by sampling directly from the coefficient file instead of the $S(\alpha,\beta,T)$ files. Results will be given in a future paper.

**Fig. 3.** Relative error in $\beta$ from true and estimated CDF for graphite, $T=887.5K$, $E=1.39E-5$ eV.

**Fig. 4.** Relative error in $\alpha$ from true and estimated CDF for graphite, $T=887.5K$, $\beta=6.36$

**CONCLUSIONS**

Functional expansions were used to fit the temperature dependence of the alpha and beta CDFs constructed from $S(\alpha,\beta,T)$ data from graphite. For the $\beta(T)$ data, second-order functional expansions in $T^{1/2}$ were used to sample beta. For the $\alpha(T)$ data, fourth-order functional expansions in $1/T$ were used to sample alpha. Both coefficient sets gave excellent results in the majority of the CDF range. The storage of coefficients is 461 kB and can be used to sample outgoing energy and angle for any incoming energy and any temperature on-the-fly. This is a large improvement from the current method which requires 24 MB of storage for each temperature. These coefficients are more compact than the current ACE data and can be combined with other on-the-fly methods in the future to complete the modeling of temperature effects for Monte Carlo codes.

**REFERENCES**