INTRODUCTION

Recently, we have developed a methodology to sample a neutron’s secondary energy and flight angle after a scattering collision adaptively in temperature in the thermal energy range [1]. This on-the-fly (OTF) method avoids the traditional sampling procedure that requires pre-storing many data at discrete temperatures. For simulations involving a large temperature variation and/or temperature feedback, the amount of pre-processing work required can be large.

The new sampling procedure takes place without recourse to the single-temperature data files. Instead, the temperature dependence of the energy ($\beta$) and momentum ($\alpha$) transfers are used to directly obtain the scattering parameters for thermal neutron scattering simulations. In order to implement this method, the probability density functions (PDFs) of the energy and momentum transfers after a collision are studied and fits are generated at cumulative distribution function (CDF) lines that best describe the temperature change using a least squares approach. The coefficients of these fits are used to perform the sampling. We have previously shown that polynomial fits using a $1/T$ basis function give the best results while only requiring a few megabytes of data storage [2]. While integral quantities like $k_{\text{eff}}$ agree well (within 1-2%) between the standard and OTF sampling methods, problems involving only a few scatters before being tallied perform poorly even if the order of the fitting is increased. This is seen for differential quantities like the secondary energy distribution. Recent work has been performed on using Monte Carlo to calculate multi-group scattering kernels for deterministic codes [3]. Incorrect sampling of the secondary thermal neutron energy when using the OTF method could result in a misrepresentation of these scattering kernels.

To improve the simulation accuracy for differential quantities, we explored a different strategy for the fitting. Instead of going for higher order in a single temperature zone, we use a lower order fitting in multiple temperature zones. The work described in this paper compares the results of generating fit coefficients by 1) using a single temperature range and 2) using various temperature zones. The former is the method that we have used in our previous studies while the latter is the new work. This new work is not applied to the secondary angle distributions since no issues have been observed with the OTF sampling of the scattering angle. The examples and results described throughout this paper use bound carbon in graphite as the material of interest.

METHOD

For solid materials like carbon bound in graphite, atoms are arranged on hexagonal lattices. The neutron interaction with a graphite lattice results in an exchange of energy that can cause the neutron to slow down (downscatter) or speed up (upscatter). In this process of energy exchanging, the various quantum mechanical modes of the crystal are changed and phonons are excited. These phonon excitations strongly affect the secondary energy distribution for a thermal neutron scattering off a solid target. In fact, certain energy transfers excite more phonons than others. These peak locations help determine which CDF probability lines should be stored when sampling thermal scattering data on-the-fly. Fig. 1 shows the distribution of phonon frequencies, $\rho(\epsilon)$, as a function of this energy transfer, $\epsilon = E' - E$ [4].

![Fig. 1. Phonon Frequency Distribution for Bound Carbon in Graphite.](image_url)

The distribution has six distinct peaks. Table I gives the beta values of the peaks for a few representative temperatures for an incident neutron energy of $1 \times 10^{-11}$ MeV, where beta is given by $\beta = \epsilon/kT$. In this table, $P1$ represents, for example, the first peak. Because of the inverse relationship between beta and temperature, the locations of the peaks are clustered around small values of beta for high temperatures and spread out to larger beta values as temperature decreases. It is important to account for the locations of the peaks and valleys in the phonon spectrum when generating thermal scattering data files [5].

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>P1</th>
<th>P2</th>
<th>P3</th>
<th>P4</th>
<th>P5</th>
<th>P6</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.6 K</td>
<td>2.168</td>
<td>3.035</td>
<td>4.335</td>
<td>5.419</td>
<td>6.070</td>
<td>6.937</td>
</tr>
<tr>
<td>600 K</td>
<td>1.061</td>
<td>1.485</td>
<td>2.121</td>
<td>2.652</td>
<td>2.970</td>
<td>3.394</td>
</tr>
<tr>
<td>1000 K</td>
<td>0.636</td>
<td>0.891</td>
<td>1.273</td>
<td>1.591</td>
<td>1.782</td>
<td>2.037</td>
</tr>
<tr>
<td>1200 K</td>
<td>0.530</td>
<td>0.742</td>
<td>1.061</td>
<td>1.326</td>
<td>1.485</td>
<td>1.697</td>
</tr>
<tr>
<td>1600 K</td>
<td>0.398</td>
<td>0.557</td>
<td>0.796</td>
<td>0.994</td>
<td>1.114</td>
<td>1.273</td>
</tr>
</tbody>
</table>

TABLE I: Beta Values at the Phonon Spectrum Peaks for $E = 1 \times 10^{-11}$ MeV ($P#$ represents the peak number).
Scattering collisions at thermal energies are sampled in Monte Carlo simulations using PDFs that account for the phonon excitations [6,7]. The energy transfer (beta) for solid scatterers is sampled from

$$\rho(\beta|E,T) = \frac{\sum_{\alpha} \exp(-\alpha \lambda) \sum_{n=0}^{\infty} \frac{1}{n!} (\alpha \lambda)^n \tau_n(\beta) d\alpha}{\sum_{\beta} \sum_{\alpha} \exp(-\alpha \lambda) \sum_{n=0}^{\infty} \frac{1}{n!} (\alpha \lambda)^n \tau_n(\beta) d\alpha d\beta},$$

where

$$\lambda = \int_{-\infty}^{\infty} \rho(\beta) \exp\left(-\frac{\beta}{2}\right) d\beta,$$

and

$$\tau_n(\beta) = \frac{kT}{2\pi \hbar^2} \int_{-\infty}^{\infty} \exp\left(-\frac{\beta kT}{\hbar}\right) \left[ \int_{-\infty}^{\infty} \rho(\beta') \exp\left(-\frac{\beta'}{2}\right) \exp\left(-\frac{\beta' kT}{\hbar}\right) d\beta' \right]^n d\beta.$$

The secondary energy is then easily calculated from the sampled beta. Traditionally, single-temperature thermal files are generated from these PDFs and used to perform the sampling. In the next sections, we describe the OTF sampling procedure and compare results using 1) a high-order single temperature zone and 2) low-order multiple temperature zones.

**SINGLE TEMPERATURE ZONE**

To sample beta and alpha (and thus $E'$ and $\mu$) adaptively in temperature, we have previously introduced a method where the PDFs in beta and alpha are converted to cumulative distribution function (CDF) form and the temperature dependence of these variables are fit along lines of equal probability. The coefficients of these fits are stored at these probability lines and used to perform the sampling for any temperature.

Results from preliminary tests show good agreement between the standard and the OTF methods for reactor applications where many scattering collisions occur. In addition, the secondary angle distribution has been shown to agree well with the new method. The secondary energy distributions, however, performed poorly due to the dominance of the phonon distribution peaks that are not present in the angular distributions. Figs. 2 and 3 show these distributions for room temperature and 1000K, respectively, for an incident neutron energy of $1 \times 10^{-11}$ MeV. In each figure, comparisons are made between the standard thermal data file and the OTF method using various polynomial orders of a $1/T$ fit.

From the figures, the higher-order polynomials perform better than the lower-order polynomials in resolving the peaks. The fitting is performed over a large range of temperatures (from 250K to 2000K) and, as a result, the fits cannot account for the sharp changes in the PDFs caused by the phonon distribution. This is better illustrated by observing how beta changes with temperature at discrete CDF lines shown in Fig. 4.

At the lower temperatures, the variation in beta with temperature indicates that a single fit for the entire temperature range will not perform well. The fits, however, pick up the “average” behavior of the PDF and the areas under the secondary energy spectra are similar between the standard and OTF methods. As a result, calculations of $k_{\text{eff}}$ agree well. Table II shows the $k_{\text{eff}}$ comparison for a VHTR fuel compact with UCO TRISO fuel in a graphite matrix. The OTF was performed with fifth-order fits in $1/T$ for the $\beta$-sampling and second-order fits in $1/T$ for...
the $\alpha$-sampling.

<table>
<thead>
<tr>
<th>Standard $S(\alpha, \beta)$</th>
<th>OTF $S(\alpha, \beta)$</th>
<th>Diff. [pcm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.6 K 1.50068(14)</td>
<td>1.50087(14)</td>
<td>19(20)</td>
</tr>
<tr>
<td>400 K 1.49885(14)</td>
<td>1.49882(13)</td>
<td>-3(19)</td>
</tr>
<tr>
<td>500 K 1.49626(14)</td>
<td>1.49631(14)</td>
<td>5(20)</td>
</tr>
<tr>
<td>600 K 1.49358(14)</td>
<td>1.49353(14)</td>
<td>-5(20)</td>
</tr>
<tr>
<td>700 K 1.49063(14)</td>
<td>1.49048(14)</td>
<td>-15(20)</td>
</tr>
<tr>
<td>800 K 1.48819(14)</td>
<td>1.48829(14)</td>
<td>10(20)</td>
</tr>
<tr>
<td>1000 K 1.48504(14)</td>
<td>1.48481(14)</td>
<td>-23(20)</td>
</tr>
<tr>
<td>1200 K 1.48129(14)</td>
<td>1.48143(14)</td>
<td>14(20)</td>
</tr>
<tr>
<td>1600 K 1.47710(14)</td>
<td>1.47726(14)</td>
<td>16(20)</td>
</tr>
</tbody>
</table>

TABLE II: Comparison of $k_{\text{eff}}$ Between Standard and OTF Methods for VHTR Fuel Compact.

In Table II, the values in parenthesis represent the standard deviation ($\sigma$) in units of pcm (1 pcm = 0.00001). The $k_{\text{eff}}$ results agree within 1-2$\sigma$ with most agreeing within 1$\sigma$. However, to obtain more accurate results for the secondary distributions, we propose a new fitting strategy. The temperature range is divided into various zones and separate fits are performed in each. The next section details this process.

MULTIPLE TEMPERATURE ZONES

The fitting procedure was performed in 11 temperature zones that better account for the sharp variations in the peaks. Table III shows this information.

<table>
<thead>
<tr>
<th>Zone #</th>
<th>Temp. Range [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>250-300</td>
</tr>
<tr>
<td>2</td>
<td>300-350</td>
</tr>
<tr>
<td>3</td>
<td>350-400</td>
</tr>
<tr>
<td>4</td>
<td>400-500</td>
</tr>
<tr>
<td>5</td>
<td>500-600</td>
</tr>
<tr>
<td>6</td>
<td>600-700</td>
</tr>
<tr>
<td>7</td>
<td>700-800</td>
</tr>
<tr>
<td>8</td>
<td>800-1000</td>
</tr>
<tr>
<td>9</td>
<td>1000-1200</td>
</tr>
<tr>
<td>10</td>
<td>1200-1600</td>
</tr>
<tr>
<td>11</td>
<td>1600-2000</td>
</tr>
</tbody>
</table>

TABLE III: Zones for Temperature Fitting.

As the temperature increases, the zones span a larger range of temperatures. This is due to the fact that the phonon peaks span a smaller range of betas at higher temperatures. To best emphasize the effect of the temperature zoning, we examine the sixth peak in the secondary energy distribution for 1000K and $E = 1 \times 10^{-11}$ MeV shown in Fig. 5.

This peak (from Table I) occurs for $\beta = 2.037$. Fig. 6 shows the beta CDF for this energy and temperature (black) compared with the CDF generated from the coefficients for no temperature zoning (from 250K-2000K) and the CDF generated from the coefficients with temperature zoning (from 1000K-1200K). In this figure, note that a fifth-order polynomial is used for the single-temperature fit and a second-order polynomial is used for the temperature zoning.

The red horizontal and vertical lines in Fig. 6 correspond to the location of the sixth peak from Fig. 5. This peak ($\beta = 2.037$) has a CDF value of around 0.91. Without the temperature zoning (pink line), it is clear that sampling CDF = 0.91 results in an undersampling of the true beta. The peak is therefore undersampled and cannot be resolved. With temperature zoning (blue), we see that the true beta value is sampled. This effect is also seen for the other peaks and at other temperatures. Figs. 7 and 8 show the distributions for room temperature and 1000K, respectively, using the new temperature zoning procedure.

In addition, the VHTR fuel compact problem [2] was run with the temperature zoning and the results are shown in Table IV. As expected, there is little difference in $k_{\text{eff}}$ whether or not temperature zoning is used.

<table>
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<td>1.47726(14)</td>
<td>16(20)</td>
</tr>
</tbody>
</table>

TABLE IV: Comparison of $k_{\text{eff}}$ Between Standard Method and Temperature-Zoning OTF Method for VHTR Fuel Compact.

Because temperature zoning requires separate sets of coef-
which exhibit strong resonance structure from the phonon spectrum currently in progress.

Fig. 7. Secondary Energy Distribution Comparison Between Standard and Various Fit Orders at Room Temperature Using Temperature Zoning.

Fig. 8. Secondary Energy Distribution Comparison Between Standard and Various Fit Orders at 1000K Using Temperature Zoning.

coefficients for each zone, the total coefficient storage increases as shown in Table V. These results are based on mesh optimization work currently in progress.

<table>
<thead>
<tr>
<th></th>
<th>(\beta) Coeffs.</th>
<th>(\alpha) Coeffs.</th>
<th>Other</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Zoning</td>
<td>0.96</td>
<td>2.51</td>
<td>1.50</td>
<td>4.97</td>
</tr>
<tr>
<td>Zoning</td>
<td>10.53</td>
<td>2.51</td>
<td>1.50</td>
<td>14.54</td>
</tr>
</tbody>
</table>

TABLE V: Coefficient Storage Size Comparison (in MB) Between Non-Zoning and Zoning Techniques.

However, because the change in the phonon peaks are not very drastic, the order of the polynomial fit can be low. For temperature zoning, we use second-order fits in \(1/T\) while fifth-order fits in \(1/T\) are used for the non-zoning approach.

It also of note to mention that temperature zoning is only necessary for solid scatterers like bound carbon in graphite which exhibit strong resonance structure from the phonon spectrum. For materials like bound hydrogen in water, the phonon spectrum is much smoother and temperature zoning is unnecessary. The total storage of coefficients for these materials are on the order of a few megabytes. Overall, the total storage size is relatively small and, at most, on the order of a single-
temperature thermal data file.

CONCLUSIONS

An OTF sampling method has been introduced recently for thermal neutron scattering and has been shown to give good results for bound carbon in graphite for \(k_{\text{eff}}\) calculations. These eigenvalues are within \(1-2\sigma\) with most falling within \(1\sigma\). A new temperature fitting technique has been presented in this paper to resolve the peaks in secondary energy spectrum plots which are of interest for those who want to perform calculations where only a few scatters occur. Although the number of temperature zones increases the amount of coefficient data needed to perform the OTF sampling, the size is still smaller than the single-temperature thermal data files currently used in Monte Carlo codes, which are on the order of 25 MB per temperature for graphite. This temperature zoning procedure makes it possible to preserve the rapid changes in peaks from the phonon excitations of the graphite lattice when performing OTF sampling of thermal scattering data.

ACKNOWLEDGMENTS

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REFERENCES