VERIFICATION OF THE ON-THE-FLY THERMAL SCATTERING SAMPLING METHOD FOR BOUND HYDROGEN IN LIGHT WATER

Andrew T. Pavlou and Wei Ji
Department of Mechanical, Aerospace & Nuclear Engineering
Rensselaer Polytechnic Institute, Troy, New York, USA
atpavlou@gmail.com
jiw2@rpi.edu

Forrest B. Brown
X Computational Physics Division
Monte Carlo Codes Group, XCP-3
Los Alamos National Laboratory, Los Alamos, New Mexico, USA
fbrown@lanl.gov

ABSTRACT

Recently, research has become very active on the fast on-the-fly (OTF) sampling of cross section data at arbitrary temperatures in Monte Carlo neutron transport simulations. This is primarily motivated by the requirement of limiting data storage in multi-physics analysis of nuclear reactors using Monte Carlo neutronic solvers. Several OTF sampling methods have been proposed, tested and reported for resolved/unresolved resonance cross section data, epithermal scattering data, and thermal scattering data. We have proposed a fast OTF sampling method to sample directly the scattered energy and angle at any temperature for thermal neutron scattering simulations. The method requires pre-processing the $S(\alpha, \beta, T)$ scattering law data and storing them into a library in a specially designed format. Monte Carlo codes can load this library to use the OTF sampling. In this paper, we report our latest progress on the verification of the method for treating bound hydrogen in light water using MCNP6. After a brief review of the basic principle and implementation of the proposed OTF method, we primarily focus on the demonstration of the method effectiveness for radiation transport simulations in three different configurations: a broomstick problem, a general light water reactor fuel pin cell, and a AP1000 fuel core model. Different neutronic quantities are calculated in these configurations including thermal scattered energy/angle distributions, eigenvalue, reactor kinetic parameters, and the neutron energy spectrum. Comparisons between the original non-OTF method and the OTF method are made. It is shown that our newly developed OTF method is highly reliable in terms of accuracy and efficiency for treating thermal scattering events with bound hydrogen in light water. The thermal data storage for bound hydrogen required by the OTF method is only about 11 MB, while current data storage libraries are about 24 MB for a single temperature.

Key Words: on-the-fly, thermal, Monte Carlo, AP1000, multi-scale, multi-physics

*Nuclear Engineering Advanced Modeling and Simulation group homepage: neams.rpi.edu
1. INTRODUCTION

High-fidelity simulations of full-core neutron transport can only be achieved with nuclear data that accounts for the possibly detailed energy and temperature changes. Monte Carlo codes typically use cross sections that are continuous in energy, but at discrete singular temperatures. Often times, changes in a reactor environment occur in the form of temperature feedback from coupling to a thermal-hydraulics code and many temperature datasets are needed. For a temperature feedback simulation, NJOY [1] could be called iteratively during the Monte Carlo process to generate the cross section data at the desired temperature. However, this has been shown to be very slow and not practical for large simulations [2]. Instead, thermal datasets are typically preprocessed before the simulation at as many temperatures as the user desires, using interpolation to obtain data at intermediate temperatures. This method becomes very memory intensive when many temperature sets are stored. In addition, accuracy is lost when interpolating between datasets to the true temperature.

Reductions in the data size have been achieved with on-the-fly (OTF) techniques; that is, a single set of temperature-independent data is pre-stored and used for the Monte Carlo simulation. Procedures during the random walk adjust these data to the changing temperatures. While these OTF methods have been shown to be successful for neutron energies much greater than 1 eV [3–8], the thermalization of neutrons at low energies makes scattering interactions difficult to model. At high neutron energies, the target atoms are treated independently; that is, as a free gas of protons with no interaction between atoms. As neutrons slow down, the thermal motion of the target nuclei significantly impacts the scattering kinematics. This thermal motion can transfer energy to the neutron during a collision causing the neutron to gain velocity. The fact that neutrons can gain or lose energy in a collision complicates the calculation of scattering kernels. More importantly, the binding of atoms in a molecule or lattice must be considered. The binding energy of atoms in a molecule is typically on the order of 1 eV and so, at higher neutron energies, these atoms can effectively be treated as unbound to their molecule and can interact freely with neutrons. As the neutron slows down, its energy becomes comparable to or less than the binding energy and the interaction mechanism is with the system of bound atoms as a whole. The scattering process changes as quantum effects become significant.

We have previously introduced a way to implement an OTF Monte Carlo technique to the double differential scattering data at thermal energies by observing the temperature dependence of the energy and momenta transfer distributions [9, 10]. These methods were shown for bound carbon in graphite. In this paper, we present preliminary work for the most widely-used moderating material of interest to the nuclear community: bound hydrogen in light water.
2. OVERVIEW OF THE ON-THE-FLY PROCESS

Perhaps the most detailed aspect of thermal neutron scattering is the inelastic portion. The double differential cross section is given by

\[ \sigma(E \rightarrow E', \mu, T) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} \exp \left( \frac{-\beta}{2} \right) S(\alpha, \beta, T), \]  

(1)

Here, \( E \) and \( E' \) represent, respectively, the incident and scattered neutron energy, \( \mu \) is the cosine of the scattering angle, \( T \) is temperature and \( \sigma_b \) is the bound microscopic scattering cross section. The variables \( \alpha \) and \( \beta \) are dimensionless quantities that define squared momentum and energy transfer, respectively,

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

(2)

Most importantly, \( S(\alpha, \beta, T) \) is the scattering law which contains information about the quantum modes and chemical binding for incoherent inelastic scattering. Unlike elastic scattering which has a straightforward temperature dependence, inelastic scattering has a complicated dependence based on the scattering law. This function does not have a smooth temperature dependence and, to use the scattering law in simulations, data processing codes pre-generate CDF tables for the scattered energy and angle based on the double differential cross section computed from the scattering law tables [11],

\[ G(\beta|E, T) = \int_{\beta_-}^{\beta_+} d\beta' \exp \left( \frac{-\beta'}{2} \right) \frac{\int_{\alpha_-}^{\alpha_+} S(\alpha, \beta', T) d\alpha}{\int_{\beta_-}^{\beta_+} \int_{\alpha_-}^{\alpha_+} \exp \left( \frac{-\beta}{2} \right) S(\alpha, \beta, T) d\alpha d\beta}, \]  

(3)

\[ H(\alpha|\beta, T) = \int_{\alpha_-}^{\alpha_+} d\alpha' \frac{S(\alpha', \beta, T)}{\int_0^\infty S(\alpha, \beta, T) d\alpha}. \]  

(4)

The OTF approach is a single set of coefficients that can be used for any temperature realization. These coefficients are solved for through a linear least squares regression by fitting the temperature dependences along discrete CDF lines [12],

\[ \begin{pmatrix} \beta(G_1, E_j, T_1) \\ \beta(G_1, E_j, T_2) \\ \vdots \\ \beta(G_i, E_j, T_P) \end{pmatrix} = \begin{pmatrix} x^0(T_1) & x^1(T_1) & \cdots & x^N(T_1) \\ x^0(T_2) & x^1(T_2) & \cdots & x^N(T_2) \\ \vdots & \vdots & \ddots & \vdots \\ x^0(T_P) & x^1(T_P) & \cdots & x^N(T_P) \end{pmatrix} \begin{pmatrix} a_{i,j,0} \\ a_{i,j,1} \\ \vdots \\ a_{i,j,N} \end{pmatrix} + \begin{pmatrix} e_{i,j,1} \\ e_{i,j,2} \\ \vdots \\ e_{i,j,P} \end{pmatrix}, \]  

(5)

\[ \begin{pmatrix} \alpha(H_k, \beta_1, T_1) \\ \alpha(H_k, \beta_1, T_2) \\ \vdots \\ \alpha(H_k, \beta_1, T_P) \end{pmatrix} = \begin{pmatrix} x^0(T_1) & x^1(T_1) & \cdots & x^M(T_1) \\ x^0(T_2) & x^1(T_2) & \cdots & x^M(T_2) \\ \vdots & \vdots & \ddots & \vdots \\ x^0(T_P) & x^1(T_P) & \cdots & x^M(T_P) \end{pmatrix} \begin{pmatrix} b_{k,l,0} \\ b_{k,l,1} \\ \vdots \\ b_{k,l,M} \end{pmatrix} + \begin{pmatrix} e_{k,l,1} \\ e_{k,l,2} \\ \vdots \\ e_{k,l,P} \end{pmatrix}. \]  

(6)

With a matrix notation representation,

\[ Y = XA + E, \]  

(7)
\( E \) represents the vector of error values from the fit. For graphite, optimization and temperature zoning techniques were invoked to determine the minimum amount of mesh points to use for the coefficients. \( x = 1/T \) basis functions were found to perform the best for the fit. These techniques were based on the unique structure of the phonon frequency spectrum of thermal excitations for crystalline-type moderators. Liquid scatterers like light water require extra considerations.

3. CONSIDERATIONS FOR LIQUID WATER

For solid scatterers like graphite, we have previously shown the phonon expansion method and its use for the calculation of the scattering law. For liquid scatterers like water, the movement of molecular clusters (translations), rotations and vibrations from the bending and stretching of the molecules must all be considered. The rotations are hindered and are treated as a solid-type mode similar to graphite. To represent the diffusive motion in water, a free-gas approximation is typically used. The combined scattering law for water excluding vibrational effects is then calculated by convolving the solid-type mode with the diffusive mode by

\[
S(\alpha, \beta, T) = S_t(\alpha, \beta, T) e^{-\alpha \lambda_s} + \int_{-\infty}^{\infty} S_t(\alpha, \beta', T)S_s(\alpha, \beta - \beta', T) d\beta'.
\]

In Equation (8), the subscripts “s” and “t” represent, respectively, the scattering law for solid-type and translational modes. The vibrational modes are treated as discrete oscillators and can also be included and convolved with the above models.

With due regard to these extra features not seen for graphite, the scattered energy \( E' \) and angle \( \mu \) are adaptively sampled in temperature with the form

\[
E'(T) \approx E + k \sum_{n=0}^{N} a_n(T)^{1-n},
\]

\[
\mu(T) \approx \frac{1}{2\sqrt{EE'}} + \left[ E + E' - A_0 k \sum_{m=0}^{2} b_m(T)^{1-m} \right],
\]

where \( N = 5 \) if no temperature zoning is used, or \( N = 3 \) with zoning. Because temperature zoning requires separate sets of coefficients for each zone, the total coefficient storage increases. Still, the total size of the coefficients is only 10.5 MB.
4. TESTING

4.1. Single-Scatter Broomstick Problem

The most sensitive type of problem to the treatment of the thermal double differential scattering mechanism is the “broomstick” benchmark [13] shown in Figure 1.

This benchmark has a fictitious geometry – it is a 1 km in length cylindrical rod with a 0.2 nm radius and a point source placed in the center. Because of the configuration, tallies can be made on neutrons that scatter only once, thus providing information about the secondary energy and angle distributions for a fixed incident neutron energy. Figures 2 and 3 show these secondary distributions for light water for an incident neutron energy of $E = 0.0253$ eV at 550K and 600K, respectively. The results are also compared with a free-gas treatment of the thermal scattering law in blue.

For both temperatures, the standard and OTF treatments compare very well with one another. There are a few angles that are slightly mis-sampled from 0 to 45 degrees. More temperature zones could be used to generate the alpha coefficients, but at the cost of data size. This slight undersampling is negligible on most general reactor neutronic simulations.
4.2. Pin Cell

The next test problem for water is a 2.0 cm tall reflecting pin cell containing uranium dioxide (UO$_2$) fuel in a zirconium clad with a water matrix. A side and overhead view of the problem geometry is shown in Figure 4.

![Figure 4. Pin cell geometry: side (left) and overhead (right) views](image)

4.2.1. $k$-eigenvalue

The eigenvalue problem was run with 50,000 source histories per cycle and 1000 active/200 inactive cycles for a total of 50 million neutron histories. To test the coefficients, the problem was run at various temperatures spanning the range of the thermal ACE files for water in order to compare with the standard ACE file lookup procedure. In addition, the importance of the $S(\alpha, \beta, T)$ treatment was...
determined by also running the benchmark at various moderator temperatures with and without the \( S(\alpha, \beta, T) \) treatment. The results are summarized in Table I. Figure 5 shows the differences between the \( S(\alpha, \beta, T) \) treatments with dashed horizontal lines representing \( \pm 2\sigma \) differences, or a 95% confidence interval. In the table, the values in parentheses are the standard deviations in units of pcm. For example, an eigenvalue of 1.00000(10) represents \( 1.00000 \pm 0.00010 \). Also, the percent relative runtime (RR) of the simulation compared to the standard \( S(\alpha, \beta, T) \) case is given by

\[
RR = 100 \left( \frac{R_{\text{off}}}{R_{\text{std}}} - 1 \right),
\]

where \( R_{\text{std}} \) and \( R_{\text{off}} \) are the runtimes for the standard and OTF simulations, respectively. Positive values indicate a slowdown while negative values represent a speedup from the standard treatment.

### Table I. Pin cell eigenvalue comparison

<table>
<thead>
<tr>
<th></th>
<th>Standard ( S(\alpha, \beta, T) )</th>
<th>On-the-Fly ( S(\alpha, \beta, T) )</th>
<th>No ( S(\alpha, \beta, T) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eigenvalue</td>
<td>RR [%]</td>
<td>Eigenvalue</td>
<td>RR [%]</td>
</tr>
<tr>
<td>293.6 K</td>
<td>1.33906(8)</td>
<td>1.33916(8)</td>
<td>+5.47</td>
</tr>
<tr>
<td>350 K</td>
<td>1.33525(8)</td>
<td>1.33510(8)</td>
<td>+5.80</td>
</tr>
<tr>
<td>400 K</td>
<td>1.33178(8)</td>
<td>1.33187(8)</td>
<td>+4.40</td>
</tr>
<tr>
<td>450 K</td>
<td>1.32861(8)</td>
<td>1.32850(7)</td>
<td>+4.78</td>
</tr>
<tr>
<td>500 K</td>
<td>1.32520(8)</td>
<td>1.32512(8)</td>
<td>+4.28</td>
</tr>
<tr>
<td>550 K</td>
<td>1.32197(8)</td>
<td>1.32187(8)</td>
<td>+4.71</td>
</tr>
<tr>
<td>600 K</td>
<td>1.31882(8)</td>
<td>1.31876(8)</td>
<td>+7.19</td>
</tr>
<tr>
<td>650 K</td>
<td>1.31595(8)</td>
<td>1.31606(8)</td>
<td>+8.36</td>
</tr>
<tr>
<td>800 K</td>
<td>1.30808(8)</td>
<td>1.30809(8)</td>
<td>+7.19</td>
</tr>
</tbody>
</table>

\( S(\alpha, \beta, T) \) has a bigger effect at low temperatures and dissipates with increasing temperature. The large difference in eigenvalue at lower temperatures indicates that \( S(\alpha, \beta, T) \) is significant for this test problem. The free atom results (i.e. no \( S(\alpha, \beta, T) \) treatment) are larger than the bound atom results due to the fact that the thermal spectrum is shifted to slightly higher energies when thermal motion is considered. This indicates that the reactivity and thus \( k_{\text{eff}} \) is smaller when using a bound atom treatment.

In comparing the two \( S(\alpha, \beta, T) \) treatments, there is a slight slowdown (around 8% at most) when running the OTF treatment, though it is relatively small. Further speedup to the new OTF sampling method is expected before permanent implementation into production Monte Carlo codes. This is saved for future work. The \( k_{\text{eff}} \) values agree very well between the standard and OTF treatments within the 95% confidence interval.
4.2.2. Temperature Coefficient of Reactivity

A simple way to observe the effect of temperature on the reactor criticality is the temperature coefficient of reactivity represented by

$$\alpha_T = \frac{\partial \rho}{\partial T} \approx \frac{\Delta \rho}{\Delta T}. \quad (11)$$

We want to ensure that $\alpha_T < 0$ because, if not, this indicates an increase in reactivity with an increase in temperature. This increase in reactivity would lead to more power, increasing the temperature further.

Table II shows the temperature coefficient of reactivity estimated from the $k$-eigenvalue results for water. Figure 6 shows the differences between the standard and OTF $S(\alpha, \beta, T)$ treatments. For all of the temperatures tested, the two methods agree within uncertainty.

<table>
<thead>
<tr>
<th>Temperature [K]</th>
<th>Standard $S(\alpha, \beta, T)$</th>
<th>On-the-Fly $S(\alpha, \beta, T)$</th>
<th>No $S(\alpha, \beta, T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\alpha_T$</td>
<td>$\delta_{\alpha_T}$</td>
<td>$\alpha_T$</td>
</tr>
<tr>
<td>321.8 K</td>
<td>-3.7782E-5</td>
<td>1.1219E-6</td>
<td>-4.0262E-5</td>
</tr>
<tr>
<td>375 K</td>
<td>-3.9027E-5</td>
<td>1.2725E-6</td>
<td>-3.6329E-5</td>
</tr>
<tr>
<td>425 K</td>
<td>-3.5831E-5</td>
<td>1.2788E-6</td>
<td>-3.8092E-5</td>
</tr>
<tr>
<td>475 K</td>
<td>-3.8735E-5</td>
<td>1.2852E-6</td>
<td>-3.8400E-5</td>
</tr>
<tr>
<td>525 K</td>
<td>-3.6875E-5</td>
<td>1.2916E-6</td>
<td>-3.7108E-5</td>
</tr>
<tr>
<td>575 K</td>
<td>-3.6135E-5</td>
<td>1.2979E-6</td>
<td>-3.5681E-5</td>
</tr>
<tr>
<td>625 K</td>
<td>-3.3074E-5</td>
<td>1.3038E-6</td>
<td>-3.1114E-5</td>
</tr>
<tr>
<td>725 K</td>
<td>-3.0480E-5</td>
<td>4.3818E-7</td>
<td>-3.0864E-5</td>
</tr>
</tbody>
</table>
Figure 6. Pin cell temperature coefficient of reactivity differences between standard and on-the-fly $S(\alpha, \beta, T)$ treatments

4.2.3. Mean Neutron Generation Time

So far, we have assumed no time dependence for the fission neutrons. In reality, some of these neutrons do not manifest themselves until after some delay. From point reactor kinetics, the time dependences of the neutron density $N$ and delayed neutron precursor concentration $C_i$ are given by

$$\frac{dN}{dt} = \left[\frac{\rho(t) - \beta}{\Lambda}\right] N(t) + \sum_{i=1}^{6} \lambda_i C_i(t), \quad (12a)$$

$$\frac{dC_i}{dt} = -\lambda_i C_i(t) + \frac{\beta_i}{\Lambda} N(t). \quad (12b)$$

Here, $\beta$ is the fraction of fission neutrons that are delayed and $\lambda$ is the precursor decay constant. We also define $\rho(t)$ as the reactivity,

$$\rho(t) = 1 - \frac{1}{k(t)}, \quad (13)$$

and $\Lambda$ as the mean generation time,

$$\Lambda = \frac{l}{k}, \quad (14)$$

where $l$ is the prompt neutron lifetime. The mean generation time is the average time between the birth of a neutron (from fission or other source) and its absorption which results in a fission event [14]. The prompt neutron lifetime is similar except the absorption does not necessarily induce fission. It is
therefore clear that these two quantities are related by the $k$-eigenvalue. MCNP [15] reports the prompt neutron lifetime, so the calculation of the mean generation time is easy to do using Eq. (14).

Table III shows the comparison of mean generation times for the different thermal scattering treatments. Figure 7 shows the differences in the mean generation times between the standard and OTF approaches. Again, the OTF method performs well.

**Table III.** Pin cell mean generation time comparison (seconds)

<table>
<thead>
<tr>
<th>Temperature [K]</th>
<th>Standard $S(\alpha, \beta, T)$</th>
<th>On-the-Fly $S(\alpha, \beta, T)$</th>
<th>No $S(\alpha, \beta, T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Lambda$</td>
<td>$\delta_{\Lambda}$</td>
<td>$\Lambda$</td>
</tr>
<tr>
<td>293.6</td>
<td>1.1890E-5</td>
<td>3.5625E-9</td>
<td>1.1875E-5</td>
</tr>
<tr>
<td>350</td>
<td>1.1875E-5</td>
<td>3.5237E-9</td>
<td>1.1871E-5</td>
</tr>
<tr>
<td>400</td>
<td>1.1868E-5</td>
<td>3.5237E-9</td>
<td>1.1858E-5</td>
</tr>
<tr>
<td>450</td>
<td>1.1858E-5</td>
<td>3.4441E-9</td>
<td>1.1863E-5</td>
</tr>
<tr>
<td>500</td>
<td>1.1852E-5</td>
<td>3.3763E-9</td>
<td>1.1848E-5</td>
</tr>
<tr>
<td>550</td>
<td>1.1846E-5</td>
<td>3.4514E-9</td>
<td>1.1852E-5</td>
</tr>
<tr>
<td>600</td>
<td>1.1842E-5</td>
<td>3.2550E-9</td>
<td>1.1837E-5</td>
</tr>
<tr>
<td>650</td>
<td>1.1818E-5</td>
<td>3.1526E-9</td>
<td>1.1816E-5</td>
</tr>
<tr>
<td>800</td>
<td>1.1817E-5</td>
<td>3.1524E-9</td>
<td>1.1816E-5</td>
</tr>
</tbody>
</table>

**Figure 7.** Pin cell mean generation time differences between standard and on-the-fly $S(\alpha, \beta, T)$ treatments.
4.2.4. Thermal Neutron Flux

It is also important to verify that the thermal neutron flux in regions containing water does not change when the OTF treatment is used since this can affect the reactor power. The flux is directly related to the reactor power by

\[
P = 3.2 \times 10^{-11} \text{[J/fission]} \times \int \int \int \sigma_f(r, E) \psi(r, E, \Omega) dV d\Omega dE
\]

where \(\sigma_f\) is the microscopic fission cross section, \(V\) is the volume, \(3.2 \times 10^{-11}\) is the average energy released per fission and \(\psi\) is the angular flux. The scalar flux is found from integration of the angular flux over angle and space. To test, the MCNP F4 tally was calculated in each water-containing cell. The F4 tally is a track-length estimate of the cell flux and has units of particles/cm\(^2\). For convenience, we express the flux per unit lethargy within each bin calculated by

\[
\phi(u_i) = E_i \phi(E_i) = \left( \frac{E_{i-1} + E_i}{2} \right) \left( \frac{F_4}{E_i - E_{i-1}} \right).
\]

Figure 8 shows the thermal neutron flux in the water moderator region for temperatures 293.6K and 800K. The standard and OTF \(S(\alpha, \beta, T)\) treatments are indistinguishable with respect to the thermal flux. The free-gas flux is also shifted slightly for both room temperature and \(T = 800\text{K}\), with the shift more predominant at room temperature. This is due to chemical binding effects which are less important at higher temperatures and energies, but critical for the lower temperatures and energies.

![Figure 8. Thermal neutron flux in water moderator region](image-url)
4.3. AP1000 Full Core

Next, we extend the analysis of the previous pin cell to a full-core geometry. Specifically, the full-core problem is modeled after the AP1000 reactor geometry [16]. The core consists of UO$_2$ pins arranged on a lattice assembly with light water as a moderator. Figure 9 shows an assembly (left) and the core arrangement of the assemblies with varying enrichments (right) [17].

![Figure 9. AP1000 fuel assembly geometry [17]](image)

The full-core problem is run with a temperature distribution using 500,000 source histories per cycle with 1000 active/200 inactive cycles. This temperature distribution is shown on the XZ plane in Table IV. The reflectors are fixed at 500K and the temperatures have a sinusoidal distribution. The temperatures used for this study were arbitrarily chosen to directly compare against the standard ACE thermal files. The results are summarized in Table V. The significance of the $S(\alpha, \beta, T)$ treatment for

| Level 10 | 450 K | 293.6 K | 350 K | 400 K | 350 K | 293.6 K | 450 K |
| Level 9  | 450 K | 350 K   | 400 K | 450 K | 400 K | 350 K   | 450 K |
| Level 8  | 450 K | 400 K   | 450 K | 500 K | 450 K | 400 K   | 450 K |
| Level 7  | 450 K | 450 K   | 500 K | 550 K | 500 K | 450 K   | 450 K |
| Level 6  | 450 K | 500 K   | 550 K | 600 K | 550 K | 500 K   | 450 K |
| Level 5  | 450 K | 500 K   | 550 K | 600 K | 550 K | 500 K   | 450 K |
| Level 4  | 450 K | 450 K   | 500 K | 550 K | 500 K | 450 K   | 450 K |
| Level 3  | 450 K | 400 K   | 450 K | 500 K | 450 K | 400 K   | 450 K |
| Level 2  | 450 K | 350 K   | 400 K | 450 K | 400 K | 350 K   | 450 K |
| Level 1  | 450 K | 293.6 K | 350 K | 400 K | 350 K | 293.6 K | 450 K |

| Reflector | 450 K | 450 K | 450 K | 450 K | 450 K | 450 K | 450 K | 450 K |
Table V. Eigenvalue and mean generation time comparisons for AP1000 full core with temperature distribution

<table>
<thead>
<tr>
<th></th>
<th>Eigenvalue</th>
<th>( \Lambda [s] )</th>
<th>RR [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard ( S(\alpha, \beta) )</td>
<td>1.20388(3)</td>
<td>2.1376E-5 ± 2.3296E-9</td>
<td>—</td>
</tr>
<tr>
<td>On-the-Fly ( S(\alpha, \beta) )</td>
<td>1.20389(3)</td>
<td>2.1382E-5 ± 2.4805E-9</td>
<td>+9.06</td>
</tr>
<tr>
<td>No ( S(\alpha, \beta) )</td>
<td>1.20548(3)</td>
<td>2.0935E-5 ± 2.2681E-9</td>
<td>−6.59</td>
</tr>
</tbody>
</table>

water is shown and the OTF treatment compares almost perfectly with the standard treatment, differing by only 1 pcm.

The thermal neutron flux was also calculated for the full core problem in the regions containing water shown in Figure 10. Again, the OTF method is able to accurately predict the thermal flux distribution compared with the standard method.

![Figure 10. Thermal neutron flux in water regions for AP1000 full core](image)

5. CONCLUSIONS

A novel method to store and sample thermal neutron scattering data has been developed for continuous-energy MC codes. This new procedure only requires the generation of fit coefficients which are applicable to any temperature, eliminating the process of pre-calculating double differential probability tables.
for the scattered energy and angle at discrete temperatures. There is a strong need for a single set of data applicable to all temperatures, specifically for multi-physics problems where there is temperature feedback from the coupling of neutronic and thermal hydraulic codes. Much like other OTF methods at higher energies, the thermal scattering fit coefficients are easy to sample from and have been shown to not slow down the MC simulation runtime significantly. For water, the coefficient size is 6.8 MB without zoning and 10.5 MB with zoning. These sizes are drastically smaller than the current storage and corrections for temperature are made during the MC random walk; data pre-processing has been eliminated.

ACKNOWLEDGMENTS

This work was supported by the RPI-NRC Nuclear Fellowship Program under the grant NRC-HQ-13-G-38-0035.

REFERENCES


