Annals of Nuclear Energy 71 (2014) 411–426

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

On-the-fly sampling of temperature-dependent thermal neutron scattering data for Monte Carlo simulations

Andrew T. Pavlou, Wei Ji *

Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, 110 8th Street, Troy, NY 12180, USA

ARTICLE INFO

Article history:
Received 23 February 2014
Accepted 22 April 2014
Available online 15 May 2014

Keywords:
On-the-fly sampling
Thermal neutron scattering
$S(\alpha,\beta)$ data
Temperature dependence
Monte Carlo simulation

ABSTRACT

Temperature can strongly affect the probabilities of certain neutron interactions (fission, capture, scattering, etc.) with materials. These probabilities are referred to in the nuclear community as 'cross sections' and are used as inputs for computer simulations. During the lifetime of a nuclear reactor, the core and its surrounding materials will experience a wide range of temperatures. To simulate the neutronic behavior in a realistic core, it is required to pre-store a large amount of cross section data to encompass the entire temperature range a neutron may experience. In recent years, methods have been developed to reduce data storage and obtain the cross section at the desired temperature 'on-the-fly' during radiation transport simulations using Monte Carlo codes. At thermal energies, however, the scattering of neutrons is complicated by their relatively small wavelengths, making molecular binding and lattice effects significant. Current approaches typically require nuclear data file sizes of tens to hundreds of MB per temperature, which can be prohibitive for realistic reactor physics simulations. To reduce the storage burden, a fitting approach in temperature is investigated that allows for the efficient evaluation of the thermal neutron scattering physics at an arbitrary temperature within a predefined range. The physics for thermal neutron scattering in graphite and hydrogen in water are evaluated with this approach. In both cases, the functional fits are able to accurately reproduce the scattering probabilities. The data storage for the fitting approach requires only a few 100 kB, which is a significant memory savings over the existing methods. These data can be used to sample a neutron's outgoing energy and scattered angle at an arbitrary temperature with minimal errors.

1. Introduction

1.1. On-the-fly sampling of nuclear data in Monte Carlo simulations

In reactor physics, nuclear reaction cross sections, as a function of neutron energy, are greatly affected by the temperature of the target material. One well-known phenomenon related to temperature effects is the Doppler broadening of cross sections at resonance neutron energies. The range of resonance energies can be broadened for fission and capture reactions as the material temperature increases due to the change in relative motion between the neutron and the target. In order to accurately model this phenomenon in the computer simulation of neutron transport and account for temperature feedback in coupled neutronic–thermal–hydraulic reactor analysis, nuclear cross sections need to be pre-calculated and stored at a wide range of temperatures. This strategy becomes ineffective as computer memory is a concern. In certain reactor designs like the Very High Temperature Gas-Cooled Reactors (VHTR), the temperature variation can be very broad and very sharp during normal and transient operations (Yesilyurt et al., 2007). This requires a prohibitive amount of memory usage to store cross section data on fine temperature bins. It is desired to seek an alternative strategy to store and use the temperature-dependent cross section data.

On-the-fly sampling is one effective means for reducing data storage in computer simulations, specifically for Monte Carlo method-based simulations. Ideally, it is desired that cross section data for neutron-nucleus reactions for any type and at any temperature can be generated and used on-the-fly during the random walk process without introducing additional computational costs compared with the pre-storage strategy. In order to achieve this, one needs to have a comprehensive understanding of physical models developed for all the cross sections evaluated and used in the past and to develop physics-based fast sampling methods that are tailored specifically for incorporation of cross sections into Monte Carlo simulations. Over the past few decades, less attention has been paid to this research area. This situation, however, has

* Corresponding author. Tel.: +1 (518) 276 6602; fax: +1 (518) 276 6025.
E-mail address: jiw2@rpi.edu (W. Ji).

http://dx.doi.org/10.1016/j.anucene.2014.04.028
0306-4549/

changed over the past few years. Recently, a method has been developed and implemented into the Monte Carlo code MCNP6 (Goorley et al., 2012) to on-the-fly sample cross sections of any reaction type for the most important resonance absorber nuclides (Yesilyurt et al., 2012). By only storing zero temperature cross sections, the Doppler broadening of total, fission and capture cross sections can be accurately sampled for the desired temperature and for any incoming neutron energy during the random walk. The computational storage has been significantly reduced by eliminating the need to store cross sections at every temperature of interest and for each isotope. Meanwhile, a new stochastic method has been developed to account for the motion of target nuclei on-the-fly by only using zero temperature cross sections in Monte Carlo neutron transport simulations. The method is based on explicit treatment of the motion of target nuclei at collision sites and the use of rejection sampling techniques. It is shown to be capable of accurately modeling continuous temperature distributions and has been implemented in the Monte Carlo reactor physics code Serpent (Viitanen and Leppänen, 2012).

For elastic scattering reactions in the epithermal energy range, new methods for the on-the-fly Doppler broadening of the elastic scattering kernel have also been developed in recent years: the Doppler Broadening Rejection Correction (DBRC) method (Becker et al., 2009) and the Weight Correction Method (WCM) (Lee et al., 2009). These methods show better accuracy than the original Sampling of the Velocity of the Target nucleus (SVT) algorithm (Carter and Cashwell, 1975) to on-the-fly sample a neutron's outgoing energy and angle after a scattering reaction at epithermal energies. Both the DBRC method and WCM involve sampling parameters in the center-of-mass frame followed by a conversion of sampled parameters back to the laboratory frame. More recently, an alternative method has been developed to directly sample a neutron's outgoing parameters in the laboratory frame with similar accuracy to the DBRC method (Sunny and Martin, 2013) by on-the-fly generating the moments of the differential scattering probability density function (PDF) at any temperature. For other important temperature-dependent cross sections, such as for scattering reactions that need to account for both thermal agitation and chemical bond effects at thermal energies and reactions at unresolved resonance energies, on-the-fly sampling methods have not yet been developed (Brown et al., 2012). In this paper, the focus is the on-the-fly sampling of $S(\alpha,\beta)$ data at thermal energies.

In previously developed on-the-fly sampling methods, the distribution of the target nuclide energy is assumed to follow a Maxwell–Boltzmann distribution. This assumption leads to the formation of analytical expressions as a function of energy and temperature for the previously studied cross sections or scattering kernel. Although these expressions are in complicated forms, such analytical temperature dependence allows the functional expansion of cross sections as a summation of a series of simple basis functions, thus providing a fast approach to generate temperature-dependent cross sections on-the-fly. However, complications arise in the thermal energy region for scattering reactions. First, the assumption of the target isotopes following a Maxwell–Boltzmann distribution is not valid. Second, neutron–nucleus scattering interactions become much more complicated than epithermal scattering and resonance reactions. Consequently, functions to account for all the physics included in the scattering event are in a complicated integral form and do not have an analytical temperature dependence (Koppel et al., 1967). This makes it much more challenging or even impossible to generate double differential scattering cross sections on-the-fly following similar methods developed for cross sections at resolved-resonance and epithermal energies. A new strategy is needed to treat the temperature dependence of the double differential scattering data in the thermal energy region. In this paper, we present an on-the-fly methodology that can sample a neutron's outgoing energy and flight angle after a thermal scattering event at an arbitrary temperature. This method removes the need to store the inelastic double differential thermal scattering cross section data at discrete temperatures.

1.2. Thermal neutron scattering with nuclear materials

When thermal neutrons interact with bound isotopes, the atom's translational, rotational and vibrational motions, which are strongly correlated with the ambient temperature, can affect the neutron scattering cross sections as well as the outgoing energy and angle after the scatter. These effects are significant for neutrons in the thermal energy range (<4 eV). In the thermal energy region, the neutron and target have comparable energies so that competing inelastic upscattering and downscattering events occur. In addition, the scattering process is divided into a coherent and an incoherent portion, where the incoherent portion ignores interference effects between the neutron and the target where the scattering from different planes of atoms can interfere as the neutron wavelength hits different atomic spacings. Both incoherent and coherent inelastic scattering are important for all moderating materials, though it is typical to ignore the coherent part of inelastic scattering with minimal error (MacFarlane et al., 2012). Therefore, the focus of this paper is on incoherent inelastic neutron scattering. Methods for temperature correcting the elastic portion of thermal neutron scattering are saved for future work.

The incoherent inelastic differential scattering cross section in the thermal region is denoted by Bischoff and Yeater (1972)

$$\sigma(E \to E', \boldsymbol{\Omega}\cdot\boldsymbol{\Omega}', T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{-\frac{\beta}{2}}S(\alpha,\beta,T), \tag{1}$$

where E and E' represent the pre- and post-collision energy, respectively, $\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}'$ represents the pre- and post-collision scattering angle ($\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}' = \mu$, where μ is the cosine of the scattering angle), σ_b is the bound atom scattering cross section, k is the Boltzmann constant (=8.617E−5 eV/K), T is the ambient temperature and $S(\alpha,\beta,T)$ is the symmetric form of the scattering law which contains much of the thermal scattering physics. The variables α and β are dimensionless quantities that define momentum and energy transfer, respectively,

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

$$\beta = \frac{E' - E}{kT}, \tag{3}$$

where A_0 is the mass ratio of the target nucleus to neutron. In classical quantum mechanics, the scattering law is related to a dynamic structure factor (Sutton et al., 2009) by

$$S(\alpha,\beta) = e^{\frac{\beta}{2}}\frac{kT}{\hbar}S(\boldsymbol{\kappa},\omega), \tag{4}$$

where $\hbar\boldsymbol{\kappa}$ and $\hbar\omega$ represent, respectively, momentum and energy transfer and $S(\boldsymbol{\kappa},\omega)$ is the dynamic structure factor. The dynamic structure factor is the time Fourier transform of the intermediate scattering function, $\chi(\boldsymbol{\kappa},t)$,

$$S(\boldsymbol{\kappa},\omega) = \frac{1}{2\pi}\int e^{-i\omega t}\chi(\boldsymbol{\kappa},t)dt, \tag{5}$$

while the intermediate scattering function is the spatial Fourier transform of a self-correlation function, $G_s(\mathbf{r},t)$,

$$\chi(\boldsymbol{\kappa},t) = \int e^{i\boldsymbol{\kappa}\cdot\mathbf{r}}G_s(\mathbf{r},t)d\mathbf{r}. \tag{6}$$

The differential self-correlation factor, $G_s(\mathbf{r},t)d\mathbf{r}$, is the conditional probability of a nucleus located in $d\mathbf{r}$ about $\mathbf{r}$ at some time t given the same nucleus located at the origin at time zero. Approx-