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Multi-group formulation of the temperature-dependent resonance scattering model and its impact on reactor core parameters

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ABSTRACT

A multi-group formulation for the exact neutron elastic scattering kernel is developed. It incorporates the neutron up-scattering effects stemming from lattice atoms thermal motion and it accounts for them within the resulting effective nuclear cross-section data. The effects pertain essentially to resonant scattering off of heavy nuclei. The formulation, implemented into a standalone code, produces effective nuclear scattering data that are then supplied directly into the DRAGON lattice physics code where the effects on Doppler reactivity and neutron flux are demonstrated. The correct accounting for the crystal lattice effects influences the estimated values for the probability of neutron absorption and scattering, which in turn affect the estimation of core reactivity and burnup characteristics. The results show an increase in values of Doppler temperature feedback coefficients up to −10% for UOX and MOX LWR fuels compared to the corresponding values derived using the traditional asymptotic elastic scattering kernel. This paper also summarizes research performed to date on this topic.

1. Introduction

The neutron slowing down equation,

$$\Sigma_t(E')\phi(E') = \int_0^\infty P(E \to E')\sigma_s(E)\phi(E)dE, \quad (1)$$

quantifies the balance of neutrons at energy E′ in an infinite domain, taking into account removal (the term on the left side of the equation) and slowing down into the energy E′, (integral term on the right side). In this equation, the slowing down term involves the scattering of neutrons from various initial energies into the energy E′, as represented by the differential scattering cross section,

$$\sigma_s(E \to E') = P(E \to E')\sigma_s(E).$$

This differential cross section is written as the product of a total scattering cross section (at energy E) and a transfer probability from E to E'. This probability inherently depends on the temperature of the scattering material. Yet, the common implementations of the solution of the neutron slowing down equation employ the temperature-independent "asymptotic scattering model" to describe the neutron-nucleus elastic scattering interactions. This "asymptotic" model, since independent of temperature, implicitly assumes that up-scattering events are ignored. Thus, in effect, rather than the equation shown above, the equation solved using traditional methods is

$$\Sigma_t(E')\phi(E') = \int_{E'}^{E'/\alpha} \frac{\sigma_s(E)}{(1-\alpha)E}\phi(E)dE. \quad (2)$$

This is tantamount to stating that the asymptotic kernel used to describe the elastic scattering transfer function is simply given by

$$\sigma_s(E)P(E \to E') = \begin{cases} \frac{\sigma_s(E)}{E(1-\alpha)}, & \alpha E \leqslant E' \leqslant E \\ 0, & otherwise \end{cases}, \quad (3)$$

where $\alpha = [(A-1)/(A+1)]^2$, in which A is the mass of the scattering nucleus in atomic mass units (amu). This scattering kernel explicitly states that neutrons starting at some energy E end with energy E' between E and αE, where α is positive and less than 1.0 and approaches zero when A is close to 1.0, i.e., when the scatterer is the nucleus of the lightest isotope of hydrogen.

The assumption of validity of the asymptotic model has been proved sufficiently accurate for neutrons scattering off of light isotopes but researchers who later questioned this theory have shown that the model is not quite as accurate for heavy nuclides with pronounced scattering resonances. The next section presents a brief review of historical developments on this subject and motivates the developments presented in this paper.

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2. A brief history of the resonance scattering model and recent developments

Until now, deterministic codes used to generate cross section data employed the asymptotic scattering model, which assumes the nucleus is at rest in the laboratory system. This assumption ignores any up-scattering events in the resonance domain. Wigner and Wilkins (1944) presented an integral equation describing the energy distribution of neutrons being slowed down uniformly throughout space by a uniformly distributed moderator whose atoms are in motion with a Maxwellian distribution of velocities. However, as they point out in their report, their formulation ignored the effects of chemical binding and crystal reflection. Blackshaw and Murray (1967) presented a new form of the scattering probability function in velocity space, assuming isotropic scattering in the center-of-mass system. In 1976, Cullen and Weisbin introduced the SIGMA1 kernel broadening method in which the cross sections are stored on a specific energy grid allowing for linear-linear interpolation between tabulated values (Cullen and Weisbin, 1976).

Ouisloumen and Sanchez (1990) first questioned the assumption made in the asymptotic scattering model (ASY) and derived a general expression (referred to here as the resonance scattering model – RSM) for temperature-dependent Legendre moments of the double differential elastic scattering cross section in a host medium characterized by a Maxwellian velocity distribution. Though their actual implementation of the model was limited to the zero-th order moment, it proved that the energy of a scattered neutron *can be* higher than the neutron energy prior to the scattering event in the resonance energy range – epithermal range. Their work also proved that the *average* neutron energy after the scattering event can be higher than the *average* energy predicted *post-event* by the asymptotic model. The same researchers also developed a Monte Carlo model and confirmed their own results (Ouisloumen, 1989). Their results revealed three important facts: (a) strong dependence of the shape of the transfer kernel on the resonance scattering cross-sections profile, i.e. the shape is far from being asymptotic when the initial neutron energy is in the vicinity of the resonance peak, particularly for the case of heavy nuclides, (b) the possibility of neutron up-scattering even at high energy, (c) strong dependence on the temperature of the scatterer target, i.e. fuel.

Later, other researchers (Kurchenkov and Laletin, 1991) proved the theoretical soundness of the model developed by Ouisloumen and Sanchez. In the mid-1990s Rothenstein and Dagan published a series of papers re-deriving the expression for the temperature-dependent transfer kernel and presenting their implementation using a stochastic methodology (Rothenstein and Dagan, 1995; Rothenstein 1996; Rothenstein and Dagan, 1998). Their papers provided a detailed explanation of the derivation of the resonance scattering model and its equivalence to the model developed by Ouisloumen and Sanchez.

In 2004, Rothenstein wrote a sequel to his previous papers, introducing a new formula to be integrated within code systems to enable the generation of $S(\alpha, \beta)$ tables (Rothenstein, 2004; Dagan, 2004). A year later in 2005 Dagan generalized the use of $S(\alpha, \beta)$ tables for ^{238}U (Dagan, 2005) and then later applied them to a burnup PWR application and reported as much as a 660 pcm change over a burnup cycle and an increase in ^{239}Pu production (Dagan and Broeders, 2006). The same method was later applied by Becker et al., 2008; Becker et al., 2009a, using MCNP (X-5 Monte Carlo Team, 2003) by preparing new $S(\alpha, \beta)$ scattering law tables and applying them to high temperature reactor (HTR) pin- and full-core calculations. They compared the use of the new scattering kernel with MCNP's standard approach ("Sampling of Velocity of Target nucleus" – SVT – which assumes the microscopic elastic scattering cross section is constant) and reported an increase in Doppler reactivity coefficient by 10% for the HTR-10 unit cells (Becker et al., 2009a), a decrease in criticality of 170–600 pcm depending on TRISO packing fraction and fuel temperature and an increase of up to 2.5% of ^{239}Pu production at end of cycle for fuel burnup. At the full-core level the same authors report a more negative Doppler reactivity by 14% and a decrease of the effective multiplication by 200–400 pcm for a model representative of the HTTR design (Becker et al., 2009a). In the same year, Becker et al. (2009b) introduced an improved Doppler broadened rejection correction (DBRC) (Becker, 2010) approach and used it to replace the approximation incorporated in MCNP concerning the scattering kernel in the resolved resonance range of heavy nuclei. The improved DBRC approach matched the results of the $S(\alpha, \beta)$ tables for heavy nuclides (presented by Dagan in 2005) to within 1–2 standard deviations with the DBRC approach increasing computation time by as much as 20%. The Doppler coefficient for their UOX fuel pin-cell model (4 $^{w}/_{o}$ ^{235}U) differed by as much as 16% when compared to the MCNP standard scattering kernel (fuel temperature range between 800 K and 1200 K). Further work by Becker et al. (2009c) applied the same methods just discussed to the Mosteller benchmark (Mosteller, 2006; Mosteller, 2007) for UOX and MOX fuel, reporting a difference of 8–16% in Doppler coefficient when compared to results obtained with the standard MCNP kernel. Likewise, when applied to a CANDU-6 model the DBRC method results in a slightly more negative fuel temperate coefficient (Dagan et al., 2011a). All the results reported by Dagan and Becker et al. were limited by applying the resonance scattering kernel only for ^{238}U and covering the energy range 10^{-5}–210 eV, thus ignoring potential effects from other nuclides and at energies outside that range.

At the same time as Becker et al. presented their results, Lee et al. (2008, 2009) applied the resonance scattering effects (via Weight Correction Method – WCM) for ^{238}U scattering data. They used Monte Carlo methods to generate the resonance integral data for CASMO-5 (Rhodes et al., 2006) and applied it to the UOX Mosteller benchmark case. Their results report a more negative fuel temperature coefficient of 9–10% (depending on the ^{235}U $^{w}/_{o}$ enrichment) and lower eigenvalues by as much as 212 pcm when compared to the asymptotic model. In the case of a HTR fuel the same researchers report a decrease in reactivity equivalent to $\sim$−450 pcm (at 1350 °C). Their results were limited to applying the resonance scattering kernel only for the ^{238}U nuclear data covering energy ranges with an upper limit of 1000 eV. The effect of the resonance scattering model and its influence on LWR reactivity initiation accidents was also studied (Grandi et al., 2010).

Likewise, later in 2009 Mori and Nagaya implemented the corrected resonance scattering model in the Monte Carlo code MVP-2 (Nagaya et al., 2005) and also applied it to the UOX Mosteller benchmark (Mori and Nagaya, 2009). They report more negative Doppler reactivity coefficients by 7.2(±0.1) to 11.7±(0.2)% (depending on the ^{235}U $^{w}/_{o}$ enrichment) when compared to the asymptotic model. Their studies included applying the corrected scattering model for energies greater than 4.5 eV and unlike previous calculations by others, applied the model to ^{238}U and ^{235}U nuclei. In 2012, Kim and Hartanto used the modified MCNP code, using Becker's DBRC method, and analyzed the fuel burnup, fuel temperature coefficient and power coefficient of reactivity for CANDU-6 (Kim and Hartanto, 2012). Zoia et al. included the DBRC and WCM techniques in the TRIPOLI-4 code, applying it to the UOX and MOX Mosteller benchmarks and performed depletions studies (Zoia et al., 2013). Hart et al. also updated the KENO Monte Carlo code, within the SCALE code system (RSICC Computer Code Collection, 2011), to include the DBRC technique (Hart et al, 2013). Further work included a burnup study (based on the DBRC technique) for