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Cross section homogenization for transient calculations in a spatially heterogeneous geometry

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ABSTRACT

The current norm in reactor accident simulation is to use homogenized cross sections that are computed using a fundamental mode flux. It is shown however, that using such cross sections in super prompt critical kinetic calculations can introduce large errors in the time dependent power. This work uses a previously developed homogenization technique (Dugan et al., 2016a), but applied to a spatially heterogeneous domain. The new homogenization method is shown to reduce the error in maximum power from ~40% when using fundamental mode homogenized cross sections to ~6% when using the new homogenization technique in the case studied. Focus is given to the time discretization used in the new homogenization technique; refinement of the temporal discretization is used to show that error reduction is possible until the point at which other sources of error dominate. Additionally, a study of the computational cost involved in this method is examined and improvements are suggested to reduce the cost incurred from using this new homogenization method.

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1. Introduction

Core calculations typically use homogenized cross sections that are generated with an equilibrium flux as the weighting function (i.e. k-eigenvalue calculation with critical leakage). Using these cross sections works well in static calculations where the flux is in the fundamental mode. However, common practice is to use these same cross sections in time dependent calculations, where the flux can vary greatly from that of the fundamental mode flux; hence reaction rates might not be preserved during the transient. It has been previously suggested that an effective homogenization weighting flux for time dependent calculations can come from an α-eigenvalue problem (Velarde et al., 1977). It has recently been shown that an instantaneous insertion of reactivity creates a shift in the energy spectrum, which can cause errors in a homogenization process (Dall'Osso, 2015). Additionally during a transient, thermal feedback effects appear that are not present in the equilibrium problem.

Previous work on time dependent homogenization (Dugan et al., 2016a) has shown that using critically homogenized cross sections for transient calculations introduces errors in the time dependent power. The previous work introduced two methods to reduce these errors and tested them with an infinite homogeneous multigroup case. The first method uses an integration of a time dependent flux as the weight function, whereas the second uses solutions of the α-eigenvalue problem as the weight function for homogenization. Further developments in this subject have applied the time integrated flux method to a spatially heterogeneous case, where the transient is initiated by a non-uniform perturbation, with 6 energy groups and an adiabatic heat model (Dugan et al., 2016b). The present work extends the work in Dugan et al. (2016b) by treating the same spatially heterogeneous case but with 26 energy groups and a multichannel heat transfer model, and studying the effects of refinement of time intervals used in the homogenization method. Additionally, the computational effort required for this homogenization method is analyzed and suggestions to reduce the cost incurred from using this new homogenization method are proposed.

2. Physical models

The analysis of accidental reactor transients involves solving at least the neutron transport and temperature distribution models during the transient; other physical models could include thermo-mechanics, power generation thermal hydraulics, and fuel stoichiometry, among others. This section describes the neutron transport and heat transfer models used to study time dependent reactor behavior, along with how these models are solved numerically when coupled in a strong manner.

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The time dependent neutron transport and delayed neutron precursor models are given by

$$\frac{\partial\vec{\psi}}{\partial t} = \underbrace{\mathbf{v}\left(\mathbf{\Sigma_s} - \mathbf{\Sigma_t} - \mathbf{L} + \mathbf{P}_\beta\mathbf{M}\right)}_{\mathbf{T}}\vec{\psi} + \mathbf{X_d}\mathbf{\Lambda}\vec{C} \tag{1}$$

$$\frac{\partial\vec{C}}{\partial t} = \boldsymbol{\mathcal{B}}\mathbf{P}\mathbf{M}\vec{\psi} - \mathbf{\Lambda}\vec{C}, \tag{2}$$

where,

$\mathbf{L}$	transport matrix $(\vec{\Omega}\cdot\vec{\nabla})$
$\mathbf{\Sigma_t}$	total cross section matrix
$\mathbf{\Sigma_s}$	scattering matrix
$\mathbf{P}$	matrix of production terms
$\mathbf{M}$	matrix which maps angular to scalar flux
$\mathbf{v}$	neutron speed
$\mathbf{X_d}$	matrix with delayed neutron spectra as columns
$\mathbf{\Lambda}$	matrix of delayed neutron decay constants
$\boldsymbol{\mathcal{B}}$	matrix of delayed neutron fractions (β_j)
$\vec{\psi}$	angular flux
$\vec{C}$	delayed neutron precursor concentration

The production matrix ($\mathbf{P} = \vec{\chi}\otimes\nu\vec{\Sigma}_f$) is made from the prompt fission spectrum ($\vec{\chi}$) and neutron production cross section ($\nu\vec{\Sigma}_f$). The matrix $\mathbf{P}_\beta$ additionally includes a delayed neutron term $(1-\beta)$ that accounts for prompt fission. Eq. (1) is accompanied by appropriate boundary and initial conditions; for the cases in this work, reflecting boundaries and a critical steady state are the accompanying conditions. Eq. (2) is accompanied by an appropriate initial condition; for this work, an equilibrium concentration corresponding to the initial flux is used. In reality, the production terms in Eqs. (1) & (2) contain a sum over fissile isotopes, which was suppressed for clarity; the sum over fissile isotopes produces delayed neutron precursors which are dependent on fissile isotope.

A 4-equation subchannel model is used to describe the thermal hydraulics of the heterogeneous lattice studied in this work. The 4-equation subchannel model is given by

$$\frac{\partial}{\partial t}\int_V \rho_x \mathrm{d}V + \int_{\partial V}\rho_x\vec{V}_x\cdot\mathrm{d}\vec{A} = -\sum_{x'}\Gamma_{x\to x'} \tag{3}$$

$$\frac{\partial}{\partial t}\int_V \rho_x\vec{V}_x\mathrm{d}V + \int_{\partial V}\vec{V}_x\rho_x\vec{V}_x\cdot\mathrm{d}\vec{A} = \vec{F}_S + \vec{F}_B \tag{4}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\int_V \rho_x e_x \mathrm{d}V + \int_{\partial V} e_x\rho_x\vec{V}_x\cdot\mathrm{d}\vec{A} = \dot{Q}_x - \dot{W}_x\\ &e_x = u + \frac{\vec{V}^2}{2} + g\Delta z,\end{aligned} \tag{5}$$

where ρ_x denotes the density, $\vec{V}_x$ is the velocity, e_x is the total energy of the thermal hydraulic species x (typically different phases of the same material). Eq. (3) requires the amount of mass within a control volume V be conserved, either through leakage on the surface or through transmutation to other species $\Gamma_{x\to x'}$. Eq. (4) states that the momentum of species x is conserved through leakage on the surface of a control volume, or by being acted on by surface and body forces, $\vec{F}_S$ and $\vec{F}_B$ respectively. Surface forces include the force due to pressure and friction between coolant and structural material, while the only body force is through gravity. Eq. (5) requires that the amount of energy within the control volume be conserved, and is added or dissipated by heat ($\dot{Q}$) or work ($\dot{W}$). The species treated with this model are liquid water and steam, and additionally a mixture species is used in Eqs. (4) & (5) to arrive at the 4-equation model. Furthermore, correlations are used to evaluate the transformation rate Γ along with forces acting on the control volume and heat and work dissipation from the control volume. The mixture species is realized through a drift velocity model between liquid and vapor water (Todreas and Kazimi, 1993). The subchannel model is achieved by discretizing the spatial domain into vertical channels, which may interchange fluid at interfaces.

The neutron transport Eq. (1) is coupled to the heat transfer model (3)–(5) through the temperature dependence of material cross sections. Material cross sections are tabulated for various water and fuel temperatures, which are interpolated during a transient to give cross sections at a specific temperature. In general, self shielding effects would need to be taken into account for each change in temperature. However, to reduce the cost of the simulations studied, it is assumed that these self shielding effects can be interpolated between temperatures. Thus, self shielding effects are computed for every state point in a reference cross section table.

The two physical models form a multiphysics system, of which a large body of recent work has been devoted to studying. Typically these models are solved as weakly coupled through a Picard-type (Tyobeka et al., 2011; Verdú et al., 2004) or a Gauss–Seidel (Kaya and Yavuz, 2000) iteration procedure among the models. However, the present work seeks to study the effect of homogenized data in the context of strong coupling between physics models. We adopt a solution approach, which has been used by much work, where the models are solved simultaneously through the construction of a single nonlinear system and obtaining the solution by Newton iterations at each time step (Charrier et al., 2003; Gaston et al., 2009; Mahadevan et al., 2012; Dugan, 2013). The nonlinear system is constructed by defining a residual equation for each physics component

$$\vec{F}(\vec{U}) = \begin{bmatrix} f_1(u_1,u_2,\ldots,u_N)\\ f_2(u_1,u_2,\ldots,u_N)\\ \vdots\\ f_N(u_1,u_2,\ldots,u_N)\end{bmatrix}, \tag{6}$$

where f_i is the residual equation and u_i is the solution for the i-th physics component. The residual system is linearized in Newton's method and minimized at each time step

$$\begin{aligned}&\mathbf{J}(\vec{U}^n)\delta\vec{U}^n = -\vec{F}(\vec{U}^n)\\ &\vec{U}^{n+1} = \vec{U}^n + \delta\vec{U}^n,\end{aligned} \tag{7}$$

where $\mathbf{J}(\vec{U}^n)$ is the Jacobian matrix for the residual system, defined as $\mathbf{J}_{ij} = \frac{\partial f_i}{\partial u_j}$. The iteration sequence in Eq. (7) is repeated until the norm of either the residual or the solution update is *sufficiently small*. A commonly used definition of *sufficiently small* is some absolute tolerance plus a fraction of the original residual size (Kelley, 1995). A Jacobian-free variant of Newton's method is used, which reduces the memory consumption (Knoll and Keyes, 2004). The Jacobian-free variant approximates the matrix–vector product, central to the Krylov linear solver used to obtain the solution update in Eq. (7), as

$$\mathbf{J}(\vec{U}^n)\vec{v} \approx \frac{\vec{F}(\vec{U}^n + \varepsilon\vec{v}) - \vec{F}(\vec{U}^n)}{\varepsilon}, \tag{8}$$

where $\vec{v}$ is a vector produced from the Krylov solver, and ε is a small parameter optimized for truncation and round-off error (An et al., 2011).