LA-UR-12-24449
Approved for public release; distribution is unlimited.

Title: Calculating Infinite-Medium alpha-Eigenvalue Spectra with a Transition Rate Matrix Method

Author(s): Betzler, Benjamin R.
Kiedrowski, Brian C.
Brown, Forrest B.
Martin, William R.

Intended for: International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, 2013-05-05/2013-05-09 (Sun Valley, Idaho, United States)

International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013)
Sun Valley, Idaho, USA, May 5-9, 2013, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2013)

CALCULATING INFINITE-MEDIUM α-EIGENVALUE SPECTRA WITH A TRANSITION RATE MATRIX METHOD

Benjamin R. Betzler
Department of Nuclear Engineering and Radiological Sciences
University of Michigan
2355 Bonisteel Boulevard, Ann Arbor, MI 48109, USA
bbetzler@umich.edu

Brian C. Kiedrowski and Forrest B. Brown
X-Computational Physics Division, Monte Carlo Codes Group
Los Alamos National Laboratory
P.O. Box 1663, MS A143 Los Alamos, NM 87545
bckiedro@lanl.gov; fbrown@lanl.gov

William R. Martin
Department of Nuclear Engineering and Radiological Sciences
University of Michigan
2355 Bonisteel Boulevard, Ann Arbor, MI 48109, USA
wrm@umich.edu

ABSTRACT

The time-dependent behavior of the energy spectrum in neutron transport was investigated with a formulation, based on continuous-time Markov processes, for computing α-eigenvalues and eigenvectors in an infinite medium. For this, a research Monte Carlo code called TORTE was created and used to estimate elements of a transition rate matrix. TORTE is capable of using both multigroup and continuous-energy nuclear data, and verification was performed. Eigenvalue spectra for infinite homogeneous mixtures were obtained and an eigenfunction expansion was used to investigate transient behavior of the neutron energy spectrum.

Key Words: Monte Carlo, time, Markov process, criticality

1. INTRODUCTION

The fission matrix method may be used to estimate k eigenvalues and eigenvectors of a system via Monte Carlo techniques [1]. The premise is that the spatial domain is discretized and transition probabilities are estimated by Monte Carlo tallies. For an adequately chosen spatial mesh, the eigenvalues and eigenvectors of the fission matrix match those of the underlying system.

The fission matrix formulation is a discrete-time Markov process where the time intervals represent fission generations. A more accurate description of temporal behavior can be obtained if the fission matrix is extended to describe transitions in continuous time. This extension models the evolution of a system as a continuous-time Markov process where the analog to the fission matrix is the transition rate matrix. A forward Monte Carlo simulation can be used to estimate elements of the transition rate matrix, similar to

how the fission matrix is estimated. The transition rate matrix can be used to define a master equation for the process, which is the Kolmogorov backward equation [2]. In the language of neutron transport, the eigenvalues of the transition rate matrix are the time-absorption or α eigenvalues, and the eigenvectors are discrete approximations of the eigenfunctions of the adjoint (backwards) transport equations.

For this paper, the discrete states are defined to be not over the spatial domain, but intervals in the energy spectrum – the geometry is assumed to be homogeneous and infinite in extent. The tallies needed to estimate elements of the transition rate matrix are defined. A standalone code called TORTE was written in MATLAB [3] capable of using either multigroup or continuous-energy nuclear data, and verification results for multigroup are presented. The results of this verification shows that, at least for infinite-medium, multigroup problems, the transition rate matrix can accurately predict α eigenvalues. Observations of continuous-energy α eigenvalue spectra are given, and, using an eigenfunction expansion, an approximation of the time-dependent behavior of the neutron energy spectrum is given. The results strongly suggest that the transition rate matrix is capable of producing accurate α-eigenvalue spectra for continuous energy as well.

2. THEORY

The Monte Carlo method performs direct simulation of neutron transport in systems. Through the use of mean values of estimators, called tallies, solutions to the neutron transport equation (which also describe mean-value neutron behavior) can be inferred. A typical assumption to handle time dependence is to assume that the temporal dimension is separable from the rest of phase space (position, energy, direction), and that the flux ψ at any time t can be described as

$$\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \sum_{n=1}^{\infty} A_n(t)\varphi_n(\mathbf{r}, E, \hat{\mathbf{\Omega}})e^{\alpha_n t}. \tag{1}$$

Here α_n is the n-th eigenvalue, φ_n is the corresponding shape eigenfunction, and A_n is an amplitude coefficient related to the neutron source. Typically of most interest is α_0, the largest or fundamental eigenvalue describing the asymptotic behavior of the system. In addition to separability, the completeness of the eigenfunctions is assumed, which has never been rigorously proven for a general system, but seems to work well empirically [4]. For a complete description in a nuclear system with fission, delayed neutron precursor rate equations must also be included. The delayed neutron precursor concentrations $C_m(\mathbf{r}, t)$ also follow exponential time behavior.

2.1. Transition Rate Matrix

The α eigenvalues and eigenfunctions can be obtained from Monte Carlo simulation by discretizing the phase space into a collection of states. For now, the spatial extent of the system is assumed to be infinite and the states denote energy intervals (or bins) or delayed neutron precursor groups. The transition rate matrix $\mathbf{Q}$ has the following form:

$$\mathbf{Q} = \begin{bmatrix} -q_{11} & q_{12} & \cdots \\ q_{21} & -q_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}. \tag{2}$$

The quantity q_{ii} is the mean net removal rate from state i, and q_{ij} ($i \neq j$) is the mean rate that neutrons transition from state i into j. Unlike typical continuous-time Markov processes, the rows are not normalized to zero, meaning there may be an overall net gain or loss in the neutron population (as would be desired in a supercritical or subcritical system).

For these calculations, $\mathbf{Q}$ is organized into four partitions: the top-left partition describes the transition of neutrons between energy intervals, the top-right partition pertains to neutrons causing fission resulting in the production of delayed neutron precursors, the bottom-left partition represents the emission of neutrons from precursors, and the bottom-right partition represents the decay (removal) of the precursors. These transition rates are expressible in terms of cross sections. In the top-left partition,

$$q_{ij} = \begin{matrix} v_i(\Sigma_{Ri} - \chi_{pi}\nu_{pi}\Sigma_{fi}), & i = j \\ v_i(\Sigma_{sij} + \chi_{pj}\nu_{pi}\Sigma_{fi}), & i \neq j \end{matrix}, \tag{3}$$

where v_i, Σ_{Ri}, Σ_{fi}, ν_{pi}, and χ_{pi} are the average speed, removal and fission cross sections, average prompt neutrons emitted per fission, and prompt fission emission probability for energy bin i; Σ_{sij} is the scattering cross section from energy bin i to j. For the top-right partition,

$$q_{ij} = v_i\beta_j\nu_{di}\Sigma_{fi}, \tag{4}$$

where β_j is the delayed fraction for precursor group j and ν_{di} is the mean delayed neutron emission for energy interval i. For the bottom-left partition,

$$q_{ij} = \chi_{ij}\lambda_i, \tag{5}$$

where χ_{ij} is the emission of neutrons from precursor group i into neutron energy interval j, and λ_i is the decay constant for precursor group i. For the bottom-right partition,

$$q_{ij} = \begin{matrix} \lambda_j, & i = j \\ 0, & i \neq j \end{matrix}. \tag{6}$$

These cross sections are identical to elements of the matrix form of the adjoint neutron transport equation. Since the adjoint eigenvalues $\alpha^\dagger$ are the complex conjugates of the forward eigenvalues α (and considering that if an eigenvalue is complex, its complex conjugate must also be an eigenvalue because the matrix is all real), then the eigenvalues of the transition rate matrix are also the α eigenvalues of the forward neutron transport equation. Unfortunately, the forward eigenvectors cannot be obtained directly from the adjoint eigenvectors, but can be obtained by taking $\mathbf{Q}^\top$, exchanging the speeds v_i and v_j, and finding the eigenvectors of the resultant matrix.

2.2. Monte Carlo Tallies

The Monte Carlo simulation is carried out as would a k-eigenvalue calculation using the power iteration technique. Technically when the system is not exactly critical, the energy spectrum is incorrect; this effect is assumed to be negligible. During the simulation, reaction rate tallies are used to estimate the q_{ij}'s.

All elements are combinations of removal rates and probabilities:

$$\lambda_i = \tau_{Ri}^{-1} = (\text{average decay time from precursor group } i)^{-1},$$

$$v_i\Sigma_{Ri} = \tau_{Ri}^{-1} = (\text{average removal time from energy interval } i)^{-1},$$

$$v_i\Sigma_{fi} = v_i\Sigma_{Ri}\frac{\Sigma_{fi}}{\Sigma_{Ri}} = \tau_{Ri}^{-1}\left(\frac{\text{\# of fissions caused by neutrons in energy interval } i}{\text{\# of removals from energy interval } i}\right),$$

$$v_i\Sigma_{sij} = v_i\Sigma_{Ri}\frac{\Sigma_{sij}}{\Sigma_{Ri}} = \tau_{Ri}^{-1}\left(\frac{\text{\# of scatters from energy interval } i \text{ into interval } j}{\text{\# of removals from energy interval } i}\right).$$

2.3. Eigenfunction Expansion Coefficients

Capturing the temporal behavior requires computing expansion coefficients $A_n(t)$ from the external source $S(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$. These are obtained from the differential equation

$$\frac{dA_n(t)}{dt} = \alpha_n A_n(t) + \frac{\left\langle \psi_n^\dagger, S \right\rangle}{\left\langle \psi_n^\dagger, v^{-1}\psi_n \right\rangle + \sum_m \left\langle C_{m,n}^\dagger, C_{m,n} \right\rangle}, \tag{7}$$

where the brackets denote integration over all relevant phase space variables.

Often, the source is a pulse at $t = 0$ or $S(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = S_0(\mathbf{r}, E, \hat{\mathbf{\Omega}})\delta(t)$ with $\delta(t)$ being the Dirac delta function. The solution simplifies to

$$A_n(t) = A_n(0)e^{\alpha_n t}, \tag{8}$$

where

$$A_n(0) = \frac{\left\langle \psi_n^\dagger, S_0 \right\rangle}{\left\langle \psi_n^\dagger, v^{-1}\psi_n \right\rangle + \sum_m \left\langle C_{m,n}^\dagger, C_{m,n} \right\rangle}. \tag{9}$$

3. CODE DESCRIPTION & VERIFICATION

TORTE is a standalone research code written in MATLAB. It is capable of performing k eigenvalue power iteration calculations with either multigroup or continuous-energy nuclear data (read from ENDF/B-VII.0 [5] or ENDF/B-VII.1 [6]). For scattering, TORTE is capable of handling both free gas and continuous $S(\alpha, \beta)$, but is limited in that it does not treat high-energy inelastic scattering. During this calculation, the aforementioned tallies for the q_{ij} are made and the α eigenvalues and eigenfunctions are estimated at the end.

Verification of the multigroup tallies was done using test problems where the multigroup cross sections are given. TORTE can reproduce the known multigroup cross sections to within 1%. Verifying the continuous-energy physics is more difficult because the results will not match production codes because high-energy inelastic scattering is excluded. Limited verification of continuous energy was done by tabulating tabulating free-gas scattering distributions and fission χ spectra and comparing them to known or analytic distributions. These comparisons agree very well.

Verification of the α eigenvalue spectrum is done with a highly-idealized problem with a known analytic solution [7]. Consider a problem where all energy groups g have the same speed v and downscattering may only occur into the next group. Fission is only possible in the lowest energy group G, which creates

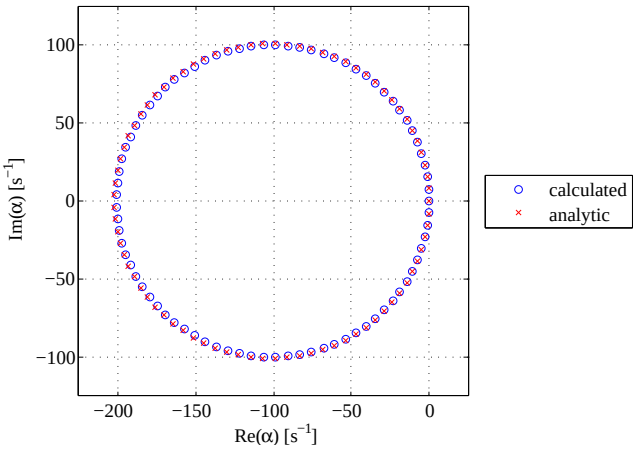


Figure 1: **The α-eigenvalue spectrum for the 81-group verification problem.**

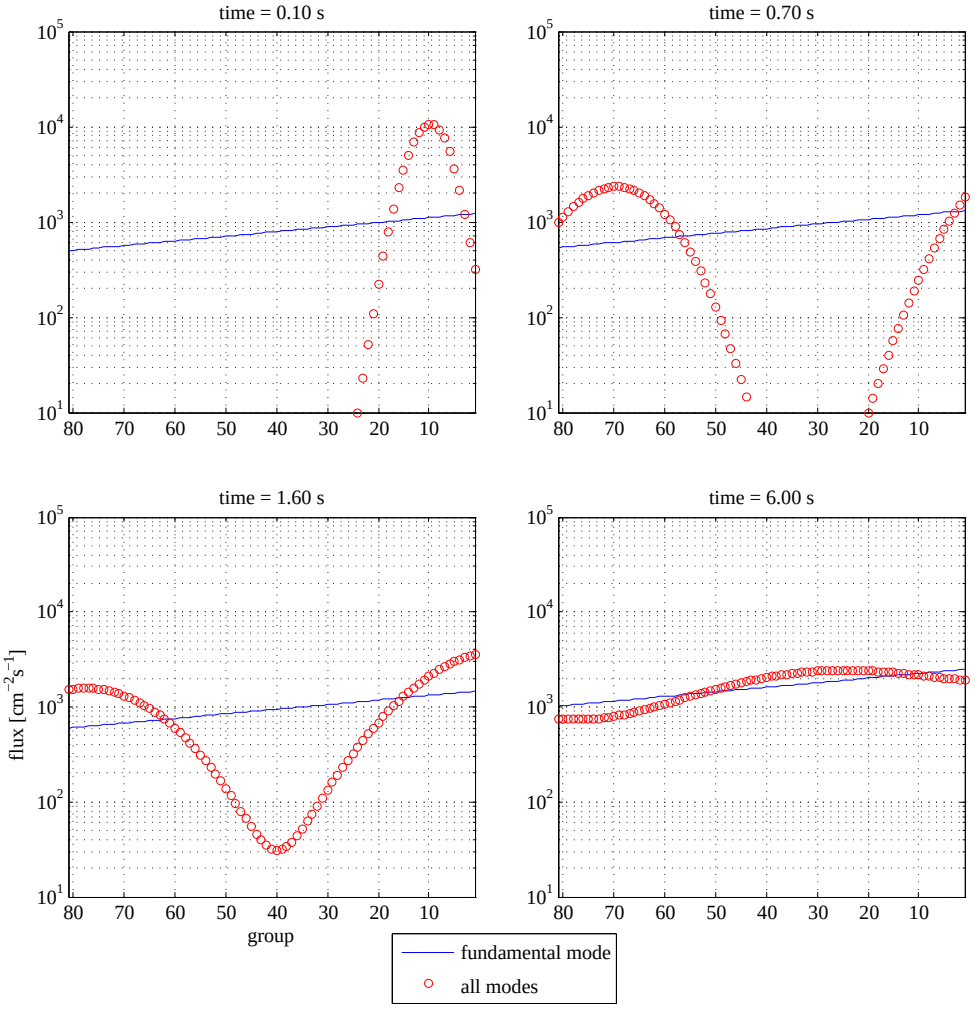


Figure 2: **Snapshots of a transient for the 81-group verification problem.**

neutrons exclusively the highest energy group, or group 1. All cross sections in all groups are identical, except for group G where the fission cross section is equal to the group-to-group scattering cross section in the other groups. The solution to this problem is a circle in the complex plane with G discrete eigenvalues given by

$$\frac{\alpha_n}{v} = -\Sigma_c + \Sigma_{sg,g+1}\left[\nu^{1/G} e^{2\pi i n/G} - 1\right]. \tag{10}$$

Arbitrary data with $G = 81$ ($\Sigma_c = 1$, $\Sigma_{fG} = \Sigma_{sg,g+1} = 100$, $v = 1$, $\nu = 2.5$) is used. The analytic and calculated eigenvalue spectra are given in Fig. 1. The two sets of results agree qualitatively. The analytic $\alpha_0 = 0.13765$ s^{-1}, whereas the calculated $\alpha_0 = 0.13839$ s^{-1}, which agrees well within 1%.

The eigenfunction expansion is tested by defining a monoenergetic ($g = 1$) pulse source, where $S_0(1) = 5 \times 10^4$ cm$^{-3} \cdot$ s^{-1}. Snapshots of the time evolution of the spectrum are given in Fig. 2: At $t = 0.10$ s, neutrons from the monoenergetic source begin to scatter out of energy group $g = 1$ at different times, resulting in a small flux packet that begins to downscatter. At $t = 0.70$ s, the flux packet continues to widen and decrease because of the different rates at which neutrons are downscattering and neutron capture. When neutrons reach energy group $g = 81$, they begin to induce fission and emit neutrons in energy group $g = 1$. At $t = 1.60$ s, the flux packet widens to the point where it combines with the neutrons fissioning into energy group $g = 1$. At $t = 6.00$ s, The flux packets are no longer discernible as the flux distribution begins to approach and follow the rising fundamental mode. As $t \to \infty$, the higher modes decay away and the complete flux solution approaches that of the fundamental mode. For this problem, this happens at $t \approx 20$ s, which is long relative to the lifetime of the prompt modes. The behavior observed here is as expected for this contrived problem.

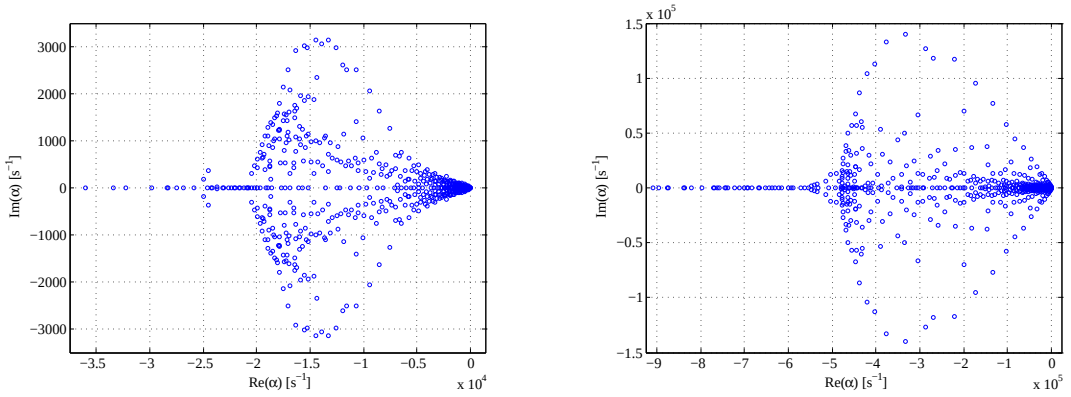
4. CONTINUOUS-ENERGY RESULTS

To understand the eigenvalue spectrum with continuous-energy nuclear data, two systems are considered: one mixture that is hydrogenous and another that is anhydrogenous (graphite moderated). These are representative of highly idealized light-water and gas-cooled, graphite-moderated reactors. Both are slightly supercritical systems with $G = 1000$ equal-lethargy bins ranging from energies $E_0 = 20$ MeV and $E_G = 1 \times 10^{-11}$ MeV. Nuclear data are obtained from ENDF/B-VII.0, except for the continuous-$S(\alpha, \beta)$ law for graphite, which is from ENDF/B-VII.1.

4.1. Hydrogenous Mixture

This is a delayed supercritical, continuous-energy, hydrogenous medium with a 4:2:1 H:O:UO_2 molecular ratio. The computed eigenvalue spectrum is given in Fig. 3a with $\alpha_0 = 1.4758 \times 10^{-3}$ s^{-1}.

Fig. 4 shows the approximated energy spectrum at selected times for a pulsed neutron source in the highest energy bin. At $t = 0.5$ ms, neutrons from the monoenergetic pulse source begin to downscatter. Flux dips form at high energies as neutrons downscatter past resonances. Because neutrons are able to downscatter to near-zero energies in a collision with hydrogen, a long tail of neutrons extends to lower energies. At $t = 1.5$ ms, neutrons continue to downscatter as the flux at high energies finally begins to dip. A very large flux packet forms. At $t = 30.0$ ms, the flux at high energies continues to decrease and dips below the fundamental mode because the neutrons downscatter out of higher energies faster than they induce fissions and emit neutrons at higher energies. Lower energy resonances cause dips in the flux packet as neutrons



(a) (b)

Figure 3: α**-eigenvalue spectra for (a) hydrogenous and (b) graphite mixtures.**

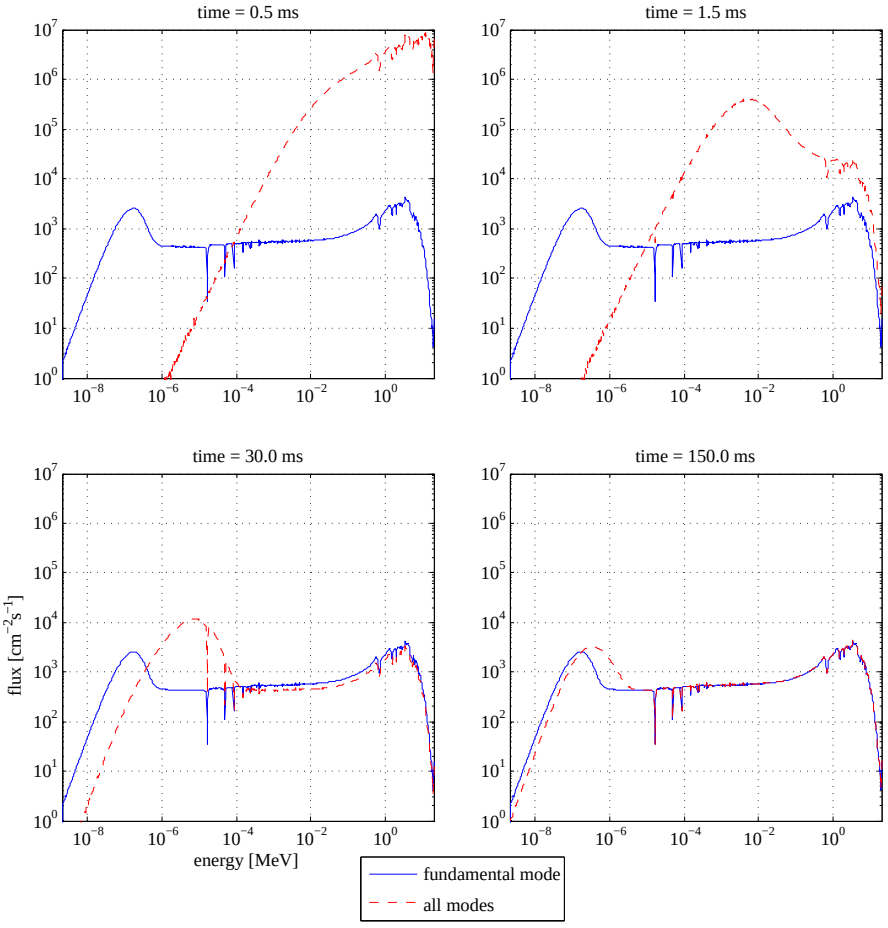


Figure 4: **Snapshots of a transient in the hydrogenous mixture.**

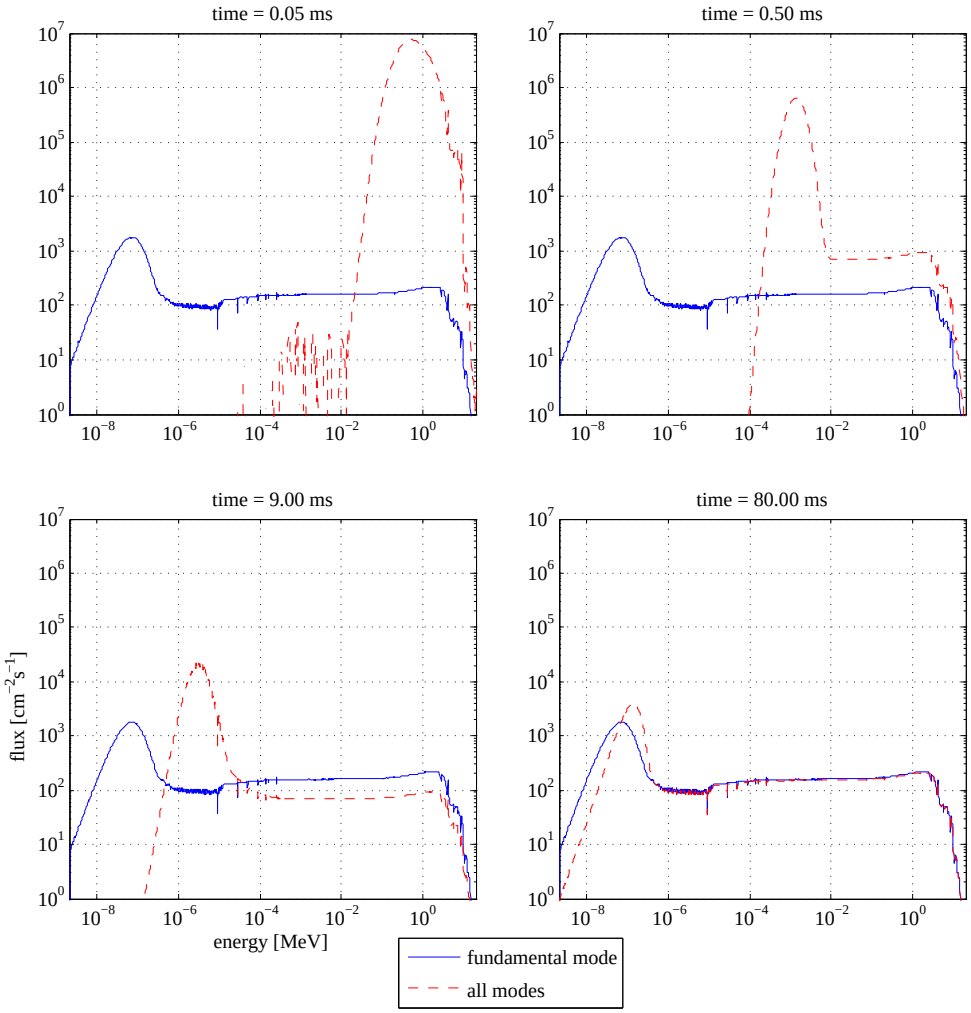


Figure 5: **Snapshots of a transient in the graphite mixture.**

downscatter. At $t = 150.0$ ms, the flux at higher energies recovers as neutrons enter thermal energies and induce fission.

4.2. Graphite Mixture

This is a highly-scattering, continuous-energy, graphite medium with a 4000:1 C:UO_2 molecular ratio. It is slightly above delayed supercritical. The calculated eigenvalue spectrum is given in Fig. 3b, where $\alpha_0 = 1.6529 \times 10^{-2}$ s^{-1}.

Fig. 5 shows the approximated energy spectrum at selected times for a pulsed neutron source in the highest energy bin. At $t = 0.05$ ms, neutrons from the monoenergetic pulse begin to downscatter and form a distinct flux packet, as neutrons colliding with carbon cannot scatter to near-zero energies. The flux at higher energies decreases rapidly, as neutrons are not at energies at which fission can replenish the higher energy flux. The peaks below the energy of the flux packet are statistical noise from the eigenfunction expansion attempting to model near-zero flux or very improbable neutrons existing at lower energies. At

$t = 0.50$ ms, the distinct flux packet maintains its form and continues to propagate to lower energies. The flux at higher energies decreases considerably and forms dips because of resonances. At $t = 9.00$ ms, the flux packet encounters low energy resonances as the flux at higher energies decreases far below the fundamental mode. Not enough neutrons induce fission because the flux packet is still above energies at which fission is preferential. At $t = 80.00$ ms, the flux at higher energies recovers because of neutrons inducing fission.

4.3. Discussion

Dips in the spectrum because of ^{238}U capture resonances are resolved with $G = 1000$. For the two mixtures, the depth of the resonance effects are different because of the vastly different relative concentrations of moderating nuclei. The flux packet is far more defined in Fig. 5 because the neutrons cannot downscatter to zero energy from carbon. This also contributes to the spectrum at higher energies decreasing below the fundamental mode more than the hydrogenous spectrum. Furthermore, the spectrum at higher energies in the graphite mixture tends to oscillate more, rising and decreasing before approaching the fundamental mode solution. This is a result of more complex eigenvalues with larger real components (relative to the fundamental) in the graphite mixture than in the hydrogenous one. The fast spectrum in the fundamental mode is also more pronounced in the hydrogenous mixture because it has a much lower concentration of scattering nuclei having a significantly harder energy spectrum.

These problems show the potential for use of eigenfunction expansion to approximate the time dependence of the energy spectrum. In both problems, the higher kinetic modes do not decay to the fundamental mode solution for a few seconds. During these first few seconds, the fundamental mode solution is a completely inaccurate representation of the energy-dependent flux shape.

5. CONCLUSIONS & FUTURE WORK

A transition rate matrix, the continuous-time analog of the fission matrix, can accurately compute α eigenvalues and eigenvectors in infinite-media. These can be applied to model transient behavior of the energy spectrum. A standalone research code called TORTE is capable of performing these calculations with either multigroup or continuous-energy nuclear data. The ability of TORTE to compute multigroup α-eigenvalue spectra has been verified, as has much of its continuous-energy scattering physics. TORTE is shown to be able to calculate continuous-energy α-eigenvalue spectra, and results have been obtained for both hydrogenous and anhydrogenous mixtures.

Future work will focus on studying the numerical convergence of the α eigenvalues and quantifying their uncertainties. Comparisons of results from TORTE will also be performed to direct, time-dependent simulations serving as further verification of the method. Finally, research will be performed to extend this method to calculate spatial modes in addition to just energy modes.

ACKNOWLEDGMENTS

Funding for this work was provided by the U.S. DOE/NNSA Advanced Scientific Computing and Nuclear Criticality Safety programs.

REFERENCES

[1] S. E. Carney, F. B. Brown, B. C. Kiedrowski, W. R. Martin, "Fission Matrix Capability for MCNP Monte Carlo," *Trans. Am. Nucl. Soc.*, **107** (2012).

[2] G. R. Grimmett, D. R. Stirzaker, *Probability and Random Processes, 3rd Ed.*, Sec. 6.9 – Continuous-time Markov chains, pp. 256-265, Oxford University Press, Oxford, UK (2001).

[3] MATLAB 7.10.0, The MathWorks Inc., Natick, MA, USA (2010).

[4] E. W. Larsen, P. F. Zweifel, "On the Spectrum of the Linear Transport Operator," *J. Math. Phys.*, **15**, No. 11, pp. 1987-1997 (1974).

[5] M. B. Chadwick, P. Obložinský, M. Herman, et al., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology,", *Nucl. Data Sheets*, **107**, pp. 2931-3060 (2006).

[6] M. B. Chadwick, M. Herman, P. Obložinský, et al., "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," *Nucl. Data Sheets*, **112**, pp. 2887-2996 (2011).

[7] E. W. Larsen, *Personal Correspondence* (2012).