

LA-UR-14-20340

Approved for public release; distribution is unlimited.

Title: Prompt Behavior of Generalized-Eigenvalue Point Kinetics Models

Author(s): Kiedrowski, Brian C.

Intended for: PHYSOR 2014, 2014-09-28/2014-10-03 (Kyoto, Japan)

Issued: 2014-01-21



Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

PROMPT BEHAVIOR OF GENERALIZED-EIGENVALUE POINT KINETICS MODELS

Brian C. Kiedrowski

X-Computational Physics Division
Los Alamos National Laboratory
P.O. Box 1663, MS A143, Los Alamos, NM 87545
bckiedro@lanl.gov

ABSTRACT

The point kinetics model is used as a first approximation for modeling transients in nuclear systems. Point kinetics is accurate enough in many situations, but its performance can degrade far from criticality. The classic approach uses a k or multiplication eigenvalue as the basis for developing the underlying model. This work generalizes the point kinetics equations for any multiplicative eigenvalue. The collision and leakage eigenvalues are studied, and preliminary results show that in some cases the collision eigenvalue provides a more accurate representation of the prompt period.

Key Words: time-dependent transport, transient, Monte Carlo, discrete ordinates

1. INTRODUCTION

The simplest model for transient behavior in a nuclear system is the point kinetics approximation[1]. Traditionally, the approximation is based upon a k or multiplication eigenvalue form of the neutron transport equation. Alternative eigenvalue formulations of the transport equation are also possible[2–5]. The point kinetics equations are reformulated to use any multiplicative eigenvalue. Using this formulation, point kinetics models based upon the collision, or c -eigenvalue, and leakage, or l -eigenvalue, are obtained.

The eigenvalue equations are identical at criticality and therefore produce identical kinetic behavior, but differ from each other for off critical systems. The suitability of using the inverse prompt period α from different point kinetics models as a surrogate for the true inverse prompt period from time-dependent transport is studied using a few multigroup systems with representative cross sections: a bare system, a fast system with a low- Z reflector, and a moderated system with a reflector. The results show that for the reflected cases, the collision c eigenvalue form of the point kinetics model does best at predicting the inverse prompt period α away from criticality.

2. THEORY

2.1. Time-Dependent Neutron Transport

The time-dependent neutron transport equation may be written as

$$\frac{1}{v} \frac{\partial \psi}{\partial t} = (S + M - L - T)\psi(\mathbf{r}, \hat{\Omega}, E, t) + \sum_i \lambda_i C_i(t) + Q(\mathbf{r}, \hat{\Omega}, E, t), \quad (1)$$

where ψ is the neutron angular flux, C_i is the delayed neutron precursor concentration for group i , v is the neutron speed, S , M , L , and T are operators for scattering, prompt fission, streaming, and total interactions respectively, λ_i is the decay constant for precursor group i , and Q is an external neutron source. The delayed neutron precursor concentrations are governed by rate equations of the following form:

$$\frac{dC_i}{dt} = B_i \psi(\mathbf{r}, \hat{\Omega}, E, t) - \lambda_i C_i(t), \quad (2)$$

where B_i is the fission production operator for delayed neutron precursors of group i .

The overall neutron population N at time t is

$$N(t) = \int \frac{1}{v} \psi(\mathbf{r}, \hat{\Omega}, E, t) d\mathbf{r} d\hat{\Omega} dE. \quad (3)$$

Often times the logarithmic rate of change in the system as a function of time is of interest,

$$\alpha(t) = \frac{1}{N(t)} \frac{dN}{dt}. \quad (4)$$

This is often referred to as dynamic α and is a general quantity describing the time behavior of an arbitrary neutronic system.

For prompt transients, the timescale of the neutron precursors is much longer than that of the rate of change of the neutron population, and those terms can be neglected. Additionally, if the external source is assumed to be of negligible intensity relative to the neutron population (as is often the case in operating nuclear reactors), then the time-dependent transport equation is

$$\frac{\partial \psi}{\partial t} = A\psi, \quad (5)$$

where $A = v(S + M - L - T)$, and is referred to as the transport operator. This equation can be formally solved via a Laplace transform, and the time-dependent solution can be obtained from the following contour integral on the complex plane:

$$\psi(\mathbf{r}, \hat{\Omega}, E, t) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{st} (s - A)^{-1} \psi_0(\mathbf{r}, \hat{\Omega}, E) ds. \quad (6)$$

Here s is the transform variable, ψ_0 is the initial condition, and γ is a constant that is sufficiently large to encompass all poles on the complex plane. Unfortunately, because of the nature of the transport operator A , the poles are not discrete points, and this contour integral is difficult[6]. Nonetheless, this assumption is often made anyway, and empirically is shown to produce good results except for the very short timescales. This allows the solution to be expressed as

$$\psi(\mathbf{r}, \hat{\Omega}, E, t) = \sum_{j=0}^{\infty} a_j e^{\alpha_j t}, \quad (7)$$

where the a_j are expansion coefficients related to the initial condition ψ_0 . The α_0 is the asymptotic inverse prompt period that is often measured experimentally in reactors, and corresponds to the dynamic α at late times assuming no delayed neutrons or sources.

It turns out that the form of a solution as a sum of exponentials may be obtained if the neutron flux is assumed to be separable from time a priori. This results in the prompt- α eigenvalue equation:

$$A\psi_\alpha = \alpha\psi_\alpha. \quad (8)$$

Here ψ_α denotes the time-independent shape function or eigenfunction, and α is the corresponding eigenvalue. The fundamental eigenvalue and eigenfunction correspond to those obtained for late times for the prompt, sourceless time-dependent neutron transport equation. The criticality condition is when the fundamental $\alpha_0 = 0$; the case where $\alpha_0 < 0$ is referred to as subcritical, and the case where $\alpha_0 > 0$ is called supercritical.

2.2. Static-Eigenvalue Equations

In practice, the time-dependent neutron transport or α -eigenvalue equations can be difficult to solve. Since behavior at or near criticality, is of most interest, the neutronic behavior can be described by a static eigenvalue equation. This is obtained by making the ad hoc assumption of steady state by setting the time derivatives to zero. Of course, the equation then does not balance unless the system was already at steady state, so a multiplicative factor is applied somewhere in the equation to enforce balance. The most popular form involves placing a factor $1/k$ on the total fission term (prompt plus delayed):

$$(L + T - S)\psi_k = \frac{1}{k}F\psi_k. \quad (9)$$

Here F is the operator for total fission, ψ_k is the shape function given this model. This is an eigenvalue problem and k is referred to as the multiplication eigenvalue, and ψ_k the corresponding eigenfunction. The k can be thought of as a factor to increase the fission multiplication uniformly to enforce balance. It follows the definition of $k = 1$ is critical, $k < 1$ is subcritical, and $k > 1$ is supercritical.

Suppose that rather than placing the multiplicative factor on the fission term, the factor $1/c$ is instead applied to the scattering plus the fission term:

$$(L + T)\psi_c = \frac{1}{c}(S + F)\psi_c. \quad (10)$$

This is the collision eigenvalue form of the transport equation, where ψ_c represents the shape function for this model, which is different than that of the k -eigenvalue model. As an aside, unlike the k eigenvalue, both the c and α eigenvalues exist even in the absence of fissionable material.

Another static-eigenvalue form of the transport equation can be created by placing a factor of $1/l$ on the total interaction term in addition to the scatter and fission terms:

$$L\psi_l = \frac{1}{l}(S + F - T)\psi_l. \quad (11)$$

Here l is the leakage eigenvalue, and corresponds to a uniform factor changing the density, or the neutron mean-free-path, to make the system critical. Unlike with the k or c eigenvalues, a positive, real l eigenvalue is not guaranteed to exist, corresponding to the situation where there is no change in material density to make the system critical.

In this study, only these three static eigenvalues are considered. One could get creative and define an infinite number of eigenvalues through different applications of multiplicative factors. In any case, for a critical configuration all of these eigenvalue equations are identical, as is the α eigenvalue equation at $\alpha_0 = 0$ and the general time-dependent transport equation. Likewise, for any multiplicative eigenvalue $x < 1$, the system is subcritical, and $x > 1$ implies the system is supercritical. There is no simple, general connection between the different static eigenvalue equations for systems that are not critical.

2.3. Adjoint Equations

The goal is to derive the point kinetics equations, but before that can be done, the adjoint equation must be introduced. The adjoint function acts as a convenient weight function allowing for simplifications to the equations. Mathematically, the adjoint function of the neutron transport equation has the following property:

$$\langle \psi^\dagger, H\zeta \rangle = \langle \zeta, H^\dagger\psi^\dagger \rangle. \quad (12)$$

Here the brackets denote integration over all phase space, H is a generic linear operator, and ζ is an arbitrary function. The adjoint function is a general, time-dependent quantity, but for brevity, only the static eigenvalue cases are considered.

The adjoint k -eigenvalue equation is

$$(L^\dagger + T^\dagger - S^\dagger) \psi_k^\dagger = \frac{1}{k} F^\dagger \psi_k^\dagger. \quad (13)$$

Here ψ^\dagger is the adjoint function of the neutron transport equation, with the daggers on the operators denoting their adjoint forms — note that $k = k^\dagger$, but the derivation of this is not shown here and available in many relevant textbooks. The adjoint equation reverses the direction of streaming, and the “direction” of scattering and fission are reversed.

The adjoint function is often given the physical meaning of importance. For the k -eigenvalue equation, this importance is the relative propensity of a neutron at some location in phase space of driving a self-sustaining chain reaction in a system where the multiplication has been adjusted by a factor of $1/k$ to make it critical.

Likewise, the collision and leakage transport equations also have corresponding adjoint equations:

$$(L^\dagger + T^\dagger) \psi_c^\dagger = \frac{1}{c} (S^\dagger + F^\dagger) \psi_c^\dagger, \quad (14)$$

$$L^\dagger \psi_l^\dagger = \frac{1}{l} (S^\dagger + F^\dagger - T^\dagger) \psi_l^\dagger. \quad (15)$$

It is also straightforward to show that $c = c^\dagger$ and $l = l^\dagger$. Furthermore, the physical interpretation of neutron importance holds, except that the physics has been adjusted in a different way for each different eigenvalue.

2.4. Generalized-Eigenvalue Point Kinetics

Now that the adjoint equations have been defined, point kinetics for a general eigenvalue x may be defined. First, group the terms in the time-dependent transport equation as follows:

$$\frac{1}{v} \frac{\partial \psi}{\partial t} = G_x \psi - H_x \psi + \sum_i \lambda_i C_i + Q, \quad (16)$$

Here G_x and H_x are operators depending on the choice of eigenvalue x from the following general eigenvalue transport equation:

$$H_x \psi_x = \frac{1}{x} (G_x + B) \psi_x, \quad (17)$$

where B is the total production operator for delayed neutrons ($M + B = F$).

From here, the point kinetics derivation proceeds in the traditional way. First, multiply the time-dependent transport equation by ψ_x^\dagger and integrate over all space.

$$\left\langle \psi_x^\dagger, \frac{1}{v} \frac{\partial \psi}{\partial t} \right\rangle = \langle \psi_x^\dagger, G_x \psi \rangle - \langle \psi_x^\dagger, H_x \psi \rangle + \sum_i \langle \psi_x^\dagger, \lambda_i C_i \rangle + \langle \psi_x^\dagger, Q \rangle, \quad (18)$$

Next, take the corresponding adjoint transport equation, multiply by ψ , and apply the property of adjoints to obtain

$$0 = \frac{1}{x} \langle \psi_x^\dagger, (G_x + B) \psi \rangle - \langle \psi_x^\dagger, H_x \psi \rangle. \quad (19)$$

Subtract this from the time-dependent equation to yield

$$\left\langle \psi_x^\dagger, \frac{1}{v} \frac{\partial \psi}{\partial t} \right\rangle = \langle \psi_x^\dagger, G_x \psi \rangle - \frac{1}{x} \langle \psi_x^\dagger, (G_x + B) \psi \rangle + \sum_i \langle \psi_x^\dagger, \lambda_i C_i \rangle + \langle \psi_x^\dagger, Q \rangle, \quad (20)$$

Add and subtract the quantity $\langle \psi_x^\dagger, B \psi \rangle$ to the right-hand side:

$$\left\langle \psi_x^\dagger, \frac{1}{v} \frac{\partial \psi}{\partial t} \right\rangle = \frac{x-1}{x} \langle \psi_x^\dagger, (G_x + B) \psi \rangle - \langle \psi_x^\dagger, B \psi \rangle + \sum_i \langle \psi_x^\dagger, \lambda_i C_i \rangle + \langle \psi_x^\dagger, Q \rangle. \quad (21)$$

Now, assume that the angular flux ψ can be separated into the fundamental mode shape function φ and a time factor $n(t)$:

$$\psi(\mathbf{r}, \hat{\Omega}, E, t) = \varphi(\mathbf{r}, \hat{\Omega}, E) n(t). \quad (22)$$

Substituting this into the equation and rearranging gives

$$\frac{dn}{dt} = \frac{\frac{x-1}{x} \langle \psi_x^\dagger, (G_x + B) \varphi \rangle - \langle \psi_x^\dagger, B \varphi \rangle}{\langle \psi_x^\dagger, \frac{1}{v} \varphi \rangle} n(t) + \sum_i \frac{\langle \psi_x^\dagger, \lambda_i C_i(t) \rangle}{\langle \psi_x^\dagger, \frac{1}{v} \varphi \rangle} + \frac{\langle \psi_x^\dagger, Q \rangle}{\langle \psi_x^\dagger, \frac{1}{v} \varphi \rangle}. \quad (23)$$

This finishes the derivation. To give a more familiar compact form, some definitions are made.

The general-eigenvalue reactivity is:

$$\rho_x = \frac{x-1}{x}; \quad (24)$$

the general-eigenvalue reproduction time is:

$$\Lambda_x = \frac{\langle \psi_x^\dagger, \frac{1}{v} \varphi \rangle}{\langle \psi_x^\dagger, (G_x + B) \varphi \rangle}; \quad (25)$$

the general-eigenvalue effective delayed neutron fraction for group i is:

$$\beta_{x,i} = \frac{\langle \psi_x^\dagger, B_i \varphi \rangle}{\langle \psi_x^\dagger, (G_x + B) \varphi \rangle}; \quad (26)$$

the general-eigenvalue effective delayed neutron fraction for all precursors is the sum of the individual components or:

$$\beta_x = \frac{\langle \psi_x^\dagger, B \varphi \rangle}{\langle \psi_x^\dagger, (G_x + B) \varphi \rangle}; \quad (27)$$

the adjoint-weighted precursor concentration for group i is:

$$c_{x,i}(t) = \frac{\langle \psi_x^\dagger, \lambda_i C_i(t) \rangle}{\langle \psi_x^\dagger, \frac{1}{v} \varphi \rangle}; \quad (28)$$

and the adjoint-weighted external source is:

$$q_x = \frac{\langle \psi_x^\dagger, Q(t) \rangle}{\langle \psi_x^\dagger, \frac{1}{v} \varphi \rangle}. \quad (29)$$

Making these definitions, the compact form of the generalized-eigenvalue point kinetics equations are obtained:

$$\frac{dn}{dt} = \frac{\rho_x - \beta_x}{\Lambda_x} n(t) + \sum_i \lambda_i c_{x,i}(t) + q_x(t), \quad (30)$$

$$\frac{dc_{x,i}}{dt} = \frac{\beta_{x,i}}{\Lambda_x} n(t) - \lambda_i c_{x,i}(t). \quad (31)$$

The inverse prompt period for the generalized-eigenvalue point kinetics equations is

$$\alpha_x = \frac{\rho_x - \beta_x}{\Lambda_x}. \quad (32)$$

For the k -eigenvalue case, this is also known as Rossi α . At criticality all values of α_x are identical and the same as the asymptotic α from the prompt-only form of the time-dependent neutron transport equation.

The shape function φ is, strictly speaking, with respect to the time-dependent transport equation. Unfortunately, that is typically not available, so a similar shape function needs to be used that is. Typically this is the neutron angular flux ψ_x for the eigenvalue problem being solved, and that is the choice made for this paper.

3. RESULTS

For this initial study, 1-D slab geometry and multigroup cross sections are used. The systems studied were a bare metal system and a metal system with a low- Z reflector. Methods for solving the forward and adjoint equations were implemented into a research discrete ordinates (S_N) code. A research Monte Carlo (MC) code was created to solve the forward and time-dependent transport problems—time dependent S_N was developed as well, but because very small time steps and negative flux fix-ups are required, MC proved to be more robust and efficient in this case. To summarize, the kinetics parameters were obtained via S_N (S_{64} Gauss-Legendre quadrature with fine spatial mesh), and the prompt α was obtained with MC by a least-squares fit to the asymptotically changing population; time cutoffs were used in the MC to control the neutron population for the supercritical cases.

As a note of verification, the S_N and MC forward eigenvalues from the two methods match, and the k eigenvalue case was benchmarked with MCNP6.1 in multigroup mode[7], providing confidence the equations are being solved correctly by both methods. As expected, the k , c , l , and time-dependent results are identical for a critical configuration. The forward and adjoint S_N eigenvalue results for k , c , and l calculations are also identical.

3.1. Bare, 2-Group Slab

Bare slabs with varying thicknesses a form the first test case. The slab cross sections are given in Table I, and the atomic density is 0.05 atoms per barn-cm. The speeds of the two groups are $v_1 = 1.0$ and $v_2 = 0.1$ in arbitrary units. For this case, no delayed neutrons were used—the 4-group case to be discussed has them.

The slab thickness a is varied from 15 to 30 cm, with the critical thickness at about 25.5 cm. Figure 1 shows the various α_x values compared with the true (reference) prompt α . For the bare case, α_k and α_c are almost identical regardless of slab thickness, whereas α_l deviates significantly from the other two away from criticality; of course, all agree at critical.

3.2. Reflected, 4-Group Slab

The next case is reflected on both sides (modeled as a reflecting boundary condition at $x = 0$). The reflector thickness on each side is 25 cm. The four energy groups are centered at 1 MeV, 100 keV, 10 eV, and 0.025 eV, so more realistic speeds are used in this case. Core and reflector cross

Table I: 2-group core cross sections.

g	σ_c	σ_f	ν	χ	σ_{sg1}	σ_{sg2}
1	1.5	1.0	2.8	1.0	0.98	0.02
2	20.0	120.0	2.5	0.0	0.00	20.0

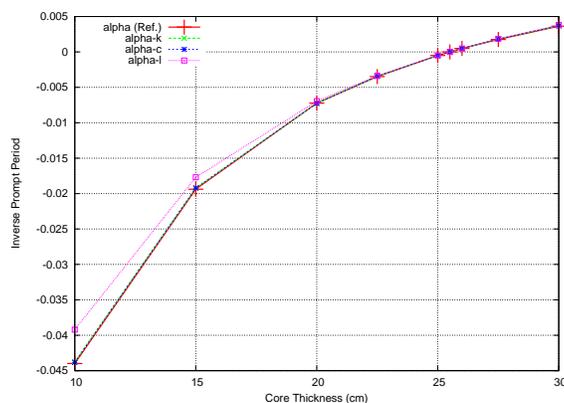


Figure 1: True α versus kinetics α_x for 2-group bare slab.

sections are given in Table II. Delayed neutrons are included with ^{235}U data used for the β_i and λ_i . To be consistent with point kinetics, only prompt ν is used to sample the fission multiplicity in the time-dependent MC calculations.

The core thickness a is varied as with the previous case. Similar comparisons of α_x and the inverse prompt period are given in Fig. 2. None of the α_x do particularly well in predicting the inverse prompt period in this case when it is far from critical. This is because the point kinetics model does not adequately insert the $1/v$ absorber or source to account for the fact that slower or faster neutrons do not significantly impact the transient. α_c is most predictive of the inverse prompt period and does better than α_k near critical; α_l is again a poor estimator of α .

Table II: 4-group core and reflector cross sections.

g	σ_c	σ_f	ν	χ_p	χ_d	σ_{sg1}	σ_{sg2}	σ_{sg3}	σ_{sg4}
1	1.5	1.0	2.8	0.8	0.7	0.7000	0.3000	0.0000	0.0000
2	0.5	1.0	2.6	0.2	0.3	0.0000	0.4998	0.0003	0.0000
3	10.0	2.0	2.5	0.0	0.0	0.0000	0.0000	4.9975	0.0025
4	20.0	120.0	2.5	0.0	0.0	0.0000	0.0000	0.0000	20.0000
1	0.2	0.0	0.0	0.0	0.0	1.1400	2.2800	0.3762	0.0038
2	0.5	0.0	0.0	0.0	0.0	0.0000	4.8000	1.1700	0.0300
3	0.5	0.0	0.0	0.0	0.0	0.0000	0.0000	4.5000	1.5000
4	1.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.2000	9.8000

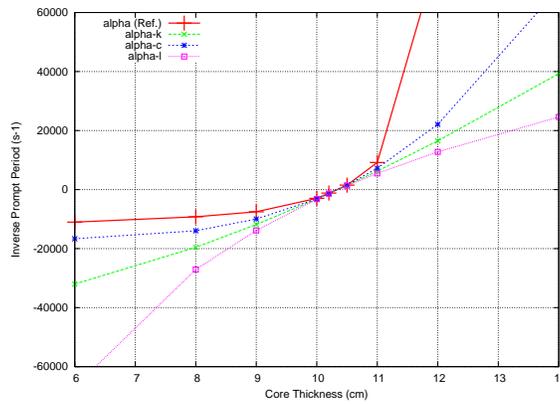


Figure 2: True α versus kinetics α_x for 4 group reflected slab.

3.3. Reflected and Moderated, 8-Group Slab

The final test problem has a similar geometry to the previous except that 8-group cross sections are used. The core of the slab is 10 thick with a 5 cm reflector on each side. The core is a mixture of fuel and moderator (reflector) material ranging from 0.2% to 40% by atom. Figure 3 gives the α results. As before, the α_c appears to offer the best approximation of the time-dependent α away from criticality; the α_k and α_l are about the same, with sometimes one performing better than the other or vice versa.

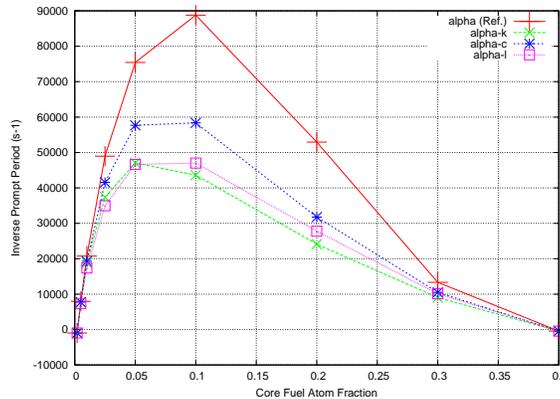


Figure 3: True α versus kinetics α_x for 8 group moderated and reflected slab.

4. SUMMARY & FUTURE WORK

The point kinetics equations were generalized to an arbitrary multiplicative static eigenvalue of the transport equation. The multiplication k , collision c , and leakage l point kinetics models were obtained from this general form and studied. Research S_N and MC codes were created to test the

ability of these models to predict the inverse prompt period α obtained from a time-dependent MC simulation. Three cases with multigroup cross sections were tested: a bare fast core (2-group), a fast core reflected by low- Z material (4-group), and a moderated core with a reflector (8-group). While it would be premature to conclude overly much based upon a few simplistic test problems using representative, but non-physical, nuclear data, the results suggest it may be worth exploring different point kinetics models, and that there may be advantages to using the c -eigenvalue kinetics for reflected systems.

The next step is to adapt these eigenvalue calculations into a continuous-energy MC code. Some of this work has already been done for the forward case with the c -eigenvalue[8]; however, new methods will need to be developed to handle the adjoint weighting needed to calculate the alternate kinetics parameters. These will most likely be logical extensions of the iterated fission probability method[9] used to compute the k point kinetics parameters.

Given the parameters from the different point kinetics models, the inhour equations may be formulated and solved. Comparisons can then be made between the models to either time dependent calculations or measurements. Finally, it may be possible to apply different combinations of these point kinetics models to multi-region kinetics, particularly regions with non-fissionable reflectors.

ACKNOWLEDGMENTS

This work was performed with support from the US DOE/NNSA Advanced Scientific Computing and Nuclear Criticality Safety Programs.

REFERENCES

- [1] G. R. Keepin, *Physics of Nuclear Kinetics*, Addison-Wesley Publishing Company, Inc., Reading, MA, USA (1965).
- [2] B. Davison, *Neutron Transport Theory*, Oxford University Press, London, UK (1958).
- [3] Y. Ronen, D. Shvarts, J. J. Wagschal, "A Comparison of Some Eigenvalues in Reactor Theory," *Nucl. Sci. Eng.*, **60**, 97-101 (1976).
- [4] G. Valarde, C. Ahnert, J. M. Aragonés, "A Comparison of the Eigenvalue Equations in k , α , λ , and γ in Reactor Theory," Nuclear Energy Agency, NEACRP-L-187 (1977).
- [5] D. C. Sahni, S. J. Sjöstrand, "Criticality and Time Eigenvalues in One-Speed Neutron Transport," *Prog. Nucl. Engrg.*, **23**, 241-289 (1990).
- [6] G. M. Wing, *An Introduction to Transport Theory*, John Wiley and Sons, Inc., New York, NY, USA (1962).
- [7] J. T. Goorley, et. al., "Initial MCNP6 Release Overview," *Nucl. Technol.*, **180** (3), 298-315 (2012).
- [8] B. C. Kiedrowski, "Evaluation of Computing c -Eigenvalues with Monte Carlo," *Trans. Am. Nucl. Soc.*, **106**, 512-515 (2012).
- [9] B. C. Kiedrowski, F. B. Brown, P. P. H. Wilson, "Adjoint-Weighted Tallies for k -Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nucl. Sci. Eng.*, **168**, 226-241 (2011).