LA-UR-10-01803

*Approved for public release; distribution is unlimited.*

*Title:* Analytic, Infinite-Medium Solutions for Point Reactor Kinetics Parameters and Reactivity Perturbations

*Author(s):* Brian C. Kiedrowski

*Intended for:* Documentation & Release Notes

# Analytic, Infinite-Medium Solutions for Point Reactor Kinetics Parameters and Reactivity Perturbations

**Brian C. Kiedrowski**
Los Alamos National Laboratory
XCP-3: Monte Carlo Codes

## 1 Introduction

Verification and validation of software and methods is vital so that users can have confidence in the results. The three methods of performing this are through comparisons of analytic solutions, results from equivalent calculations with other numerical methods, and experimental data. The advantage of an analytic solution (assuming that it, in itself, is correct) is that there is no question of the veracity of the benchmark result. Method and experimental comparisons, however, have potential issues of approximations and errors in software and biases in measurements and instrumentation. Unfortunately, analytic solutions are typically only available for idealized, simple (and sometimes, arguably trivial) problems. Therefore, the other two approaches of validation and verification are utterly indispensable.

Infinite medium solutions for comparing the kinetics parameters and reactivity changes are provided. The advantage of an infinite medium problem is that a solution to the transport equation can usually be obtained algebraically without resort to the techniques of calculus. Of course, such solutions lack any notion of geometric effect and, therefore, cannot be viewed as a complete verification. Nonetheless, while spatial effects cannot be captured, spectral ones can. This, in and of itself, makes an infinite medium solution useful.

## 2 Analytic Kinetics Solutions

The neutron generation time has the following formulation:

$$\Lambda = \frac{\langle \psi^\dagger, v^{-1}\psi \rangle}{\langle \psi^\dagger, F\psi \rangle}. \tag{1}$$

The brackets denote an integration over all space, energy, and direction. For an infinite medium solution, the space and direction components are uniform, so for these solutions, it will merely be a sum over energy. The nomenclature is as follows: $\psi$ is the forward angular flux, $\psi^\dagger$ is the adjoint angular flux, $v$ is the neutron speed, and $F$ is the operator for prompt fission, which has the following form:

$$F = \frac{\chi_p(E)}{4\pi} \iint dE' d\Omega' \nu \Sigma_f(E). \tag{2}$$

Additionally, $\chi$ is the energy dependent prompt emission spectrum, $\nu$ is the average number of neutrons per fission that is usually grouped with $\Sigma_f$, the macroscopic fission cross section. Note that for these problems, since the angular flux is isotropic, the factors of $4\pi$ will be suppressed.

### *One-Group Generation Time*

For one-group, the solutions are very simple. The forward equation takes the following infinite medium form:

$$\Sigma_t \psi = \Sigma_s \psi + \frac{1}{k_\infty} \nu \Sigma_f \psi. \tag{3}$$

$\Sigma_t$ is the total macroscopic cross section, $\Sigma_s$ is the isotropic scattering cross section, and $k_\infty$ is the eigenvalue for an infinite medium. Define the macroscopic absorption cross section as $\Sigma_a = \Sigma_t - \Sigma_s$. The eigenvalue is then

$$k_\infty = \frac{\nu \Sigma_f}{\Sigma_a}. \tag{4}$$

For these problems, it will be assumed that nuclear data will be selected to make $k_\infty = 1$. The analytic solution for $\Lambda$ is also easy to obtain because all terms can be factored:

$$\Lambda = \frac{1}{v\nu\Sigma_f}. \tag{5}$$

***Two-Group Generation Time***

A one-group solution of $\Lambda$, being the simplest possible solution, is almost trivial since the forward and adjoint fluxes are identical. It would be more instructive to perform a two-group problem. For simplicity, it will be assumed that there is no upscatter and fission neutrons are born into group 1. In principle, it is possible to find more generalized solutions as well.

The forward equation for group 1 takes the form:

$$\Sigma_{t1}\psi_1 = \Sigma_{s11}\psi_1 + \frac{1}{k_\infty}\left(\nu\Sigma_{f1}\psi_1 + \nu\Sigma_{f2}\psi_2\right). \tag{6}$$

The numerical subscripts denote that the cross section applies to that energy group. The cross section $\Sigma_{sg'g}$ is the scattering cross section for neutrons in group $g'$ transferring to group $g$. It is also useful to define the removal cross section for group $g$ as: $\Sigma_{Rg} = \Sigma_{tg} - \Sigma_{sgg}$. From here, it is possible to manipulate (6) to solve for the eigenvalue:

$$k_\infty = \frac{\nu\Sigma_{f1}}{\Sigma_{R1}} + \frac{\nu\Sigma_{f2}}{\Sigma_{R1}}\frac{\psi_2}{\psi_1}. \tag{7}$$

The ratio of $\psi_2$ to $\psi_1$ remains unknown. To find this, write the forward equation for group 2:

$$\Sigma_{t2}\psi_2 = \Sigma_{s22}\psi_2 + \Sigma_{s12}\psi_1. \tag{8}$$

The ratio is

$$\frac{\psi_2}{\psi_1} = \frac{\Sigma_{s12}}{\Sigma_{R2}}. \tag{9}$$

By substitution of (9) into (7), the eigenvalue is solved:

$$k_\infty = \frac{\nu\Sigma_{f1}}{\Sigma_{R1}} + \frac{\nu\Sigma_{f2}}{\Sigma_{R2}}\frac{\Sigma_{s12}}{\Sigma_{R1}}. \tag{10}$$

The adjoint equations for groups 1 and 2 are:

$$\Sigma_{t1}\psi_1^\dagger = \Sigma_{s11}\psi_1^\dagger + \Sigma_{s12}\psi_2^\dagger + \nu\Sigma_{f1}\psi_1^\dagger, \tag{11}$$

$$\Sigma_{t2}\psi_2^\dagger = \Sigma_{s22}\psi_2^\dagger + \nu\Sigma_{f2}\psi_1^\dagger. \tag{12}$$

Like with the forward solution, it is possible to find a ratio of adjoint fluxes:

$$\frac{\psi_1^\dagger}{\psi_2^\dagger} = \frac{\Sigma_{R2}}{\nu\Sigma_{f2}}. \tag{13}$$

Since eigenvalue problems have an extra degree of freedom for both the forward and adjoint equations, some value must be defined somewhere to have a unique solution. Note that this does not impact the magnitude of any ratio quantity such as the neutron generation time. A convenient choice is: $\psi_1 = 1$ and $\psi_2^\dagger = 1$. From these specification, it is possible to easily solve for $\Lambda$. The numerator has the form:

$$\left\langle \psi^\dagger, v^{-1}\psi \right\rangle = \psi_1^\dagger \frac{1}{v_1}\psi_1 + \psi_2^\dagger \frac{1}{v_2}\psi_2 = \frac{1}{v_1}\frac{\Sigma_{R2}}{\nu\Sigma_{f2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}}. \tag{14}$$

It follows that the denominator is:

$$\left\langle \psi^\dagger, F\psi \right\rangle = \psi_1^\dagger\left(\nu\Sigma_{f1}\psi_1 + \nu\Sigma_{f2}\psi_2\right) = \frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12}. \tag{15}$$

By taking the ratio of (14) and (15), the neutron generation time is obtained:

$$\Lambda = \frac{\frac{1}{v_1}\frac{\Sigma_{R2}}{\nu\Sigma_{f2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}}}{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12}}. \tag{16}$$

***Two-Group Effective Delayed Neutron Fraction***

The effective delayed neutron fraction has the following expression:

$$\beta_{\text{eff}} = \frac{\langle \psi^\dagger, B\psi \rangle}{\langle \psi^\dagger, F\psi \rangle}. \tag{17}$$

$F$ is now the operator for total fission, and $B$ is the operator for the delayed component. The operator for total fission is,

$$F = \frac{1}{4\pi}\iint dE'd\Omega' \left[(1-\beta)\chi_p(E) + \sum_i \beta_i \chi_i(E)\right]\nu\Sigma_f(E). \tag{18}$$

Here $\beta$ denotes the total delayed neutron fraction which is the sum of the individual fractions $\beta_i$ for each precursor group $i$. The total delayed neutron fraction $\beta$ should not be confused with the effective delayed neutron fraction $\beta_{\text{eff}}$. The former is a fundamental constant of the universe in that a neutron of particular incident energy upon a specific nucleus will produce (on average) some fraction of precursor fission products, which, in turn, emit delayed neutrons. The effective delayed neutron is a property related to a specific system involving an importance weighted average of fission neutrons.

There will be some simplifications to make the problem easier to solve. First, emission spectra will be independent of incident energy. Secondly, the delayed neutron fractions will also be independent of energy. For additional nomenclature, $\chi_{pg}$ and $\chi_{ig}$ are the prompt and delayed (of precursor $i$) emission spectra for energy group $g$. To simplify notation, $\xi_g$ will be the sum of all $\chi_{ig}\beta_i$. As a further simplification, the prompt neutrons will only be emitted in group 1 such that $\chi_{p1} = 1$. Delayed neutrons, however, can be emitted into both groups. Finally, only neutrons in group 2 may cause fission ($\nu\Sigma_{f2} = \nu\Sigma_f$) and there is no upscatter.

From here, it is possible to write the forward equations:

$$\Sigma_{t1}\psi_1 = \Sigma_{s11}\psi_1 + \frac{1}{k_\infty}\left[(1-\beta) + \xi_1\right]\nu\Sigma_f\psi_2, \tag{19}$$

$$\Sigma_{t2}\psi_2 = \Sigma_{s22}\psi_2 + \Sigma_{s12}\psi_1 + \frac{1}{k_\infty}\xi_2\nu\Sigma_f\psi_2. \tag{20}$$

$k_\infty$ may be obtained from (19):

$$k_\infty = \left[(1-\beta) + \xi_1\right]\frac{\nu\Sigma_f}{\Sigma_{R1}}\frac{\psi_1}{\psi_2}. \tag{21}$$

With equation (20), the flux ratio is

$$\frac{\psi_2}{\psi_1} = \frac{\Sigma_{s12}}{\Sigma_{R2} - \frac{1}{k_\infty}\xi_2\nu\Sigma_f}. \tag{22}$$

By substituting (22) into (21) and rearranging, the eigenvalue can be obtained:

$$k_\infty = \left[(1-\beta) + \xi_1\right]\frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R1}\Sigma_{R2}} + \frac{\xi_2\nu\Sigma_f}{\Sigma_{R2}}. \tag{23}$$

The adjoint equations are:

$$\Sigma_{t1}\psi_1^\dagger = \Sigma_{s11}\psi_1^\dagger + \Sigma_{s12}\psi_2^\dagger, \tag{24}$$

$$\Sigma_{t2}\psi_2^\dagger = \Sigma_{s22}\psi_2^\dagger + \nu\Sigma_f\left\{\left[(1-\beta) + \xi_1\right]\psi_1^\dagger + \xi_2\psi_2^\dagger\right\}. \tag{25}$$

From (24) the ratio of adjoint fluxes is obtained:

$$\frac{\psi_1^\dagger}{\psi_2^\dagger} = \frac{\Sigma_{s12}}{\Sigma_{R1}}. \tag{26}$$

Again, defining $\psi_1 = 1$ and $\psi_2^\dagger = 1$, it is possible to solve for the terms in $\beta_{\text{eff}}$. The numerator is:

$$\left\langle \psi^\dagger, B\psi \right\rangle = \left(\xi_1\psi_1^\dagger + \xi_2\psi_2^\dagger\right)\nu\Sigma_f\psi_2. \tag{27}$$

Likewise, the denominator is

$$\left\langle \psi^\dagger, F\psi \right\rangle = \left\{\left[(1-\beta)+\xi_1\right]\psi_1^\dagger + \xi_2\psi_2^\dagger\right\}\nu\Sigma_f\psi_2. \tag{28}$$

By taking the ratio and substituting in for the adjoint fluxes, the effective delayed neutron is obtained:

$$\beta_{\text{eff}} = \frac{\frac{\Sigma_{s12}}{\Sigma_{R1}}\xi_1 + \xi_2}{\frac{\Sigma_{s12}}{\Sigma_{R1}}\left[(1-\beta)+\xi_1\right] + \xi_2}. \tag{29}$$

***Two-Group Rossi-Alpha***

Rossi-$\alpha$ is defined as

$$\alpha = -\frac{\beta_{\text{eff}}}{\Lambda}. \tag{30}$$

By manipulation of (1) and (17), Rossi-$\alpha$ is

$$\alpha = -\frac{\left\langle \psi^\dagger, B\psi \right\rangle}{\left\langle \psi^\dagger, v^{-1}\psi \right\rangle}. \tag{31}$$

The two-group problem from the $\beta_{\text{eff}}$ calculation will be used. The numerator is the same as before and is given in (27). The denominator can be done through substitution:

$$\left\langle \psi^\dagger, v^{-1}\psi \right\rangle = \frac{1}{v_1}\frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2} - \xi_2\nu\Sigma_f}. \tag{32}$$

By taking the ratio, Rossi-$\alpha$ is obtained:

$$\alpha = -\frac{\left[\frac{\Sigma_{s12}}{\Sigma_{R1}}\xi_1 + \xi_2\right]\frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}}{\frac{1}{v_1}\frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}}. \tag{33}$$

## 3 Analytic Perturbation Solutions

The change in reactivity $\rho$ from a small change in a system configuration can be found, to first order, using perturbation theory:

$$\rho = -\frac{\left\langle \psi^\dagger, \left(\Delta\Sigma_t - \Delta S - \lambda\Delta F\right)\psi \right\rangle}{\left\langle \psi^\dagger, F'\psi \right\rangle}. \tag{34}$$

From left to right, the terms in the numerator, when acting on the flux, are: the change in the total collision rate, the change in the scattering source, and the change in the fission source. Note that $\lambda = 1/k_\infty$ and is taken to be unperturbed. The denominator has the perturbed fission source $F'$ acting upon the flux. Any term with that is perturbed will be primed.

The new eigenvalue from perturbation theory $\tilde{k}'_\infty$ can be found from the reactivity:

$$\tilde{k}'_\infty = \frac{1}{\lambda - \rho}. \tag{35}$$

Also, the ratio of perturbed to exact $P/E$ can be found if the analytic solution of $k'$ is known as well by taking the ratio:

$$P/E = \tilde{k}'_\infty / k'_\infty. \tag{36}$$

***Generalized One-Group Perturbation***

Suppose each term in (34) is perturbed for a monoenergetic, homogeneous, and infinite system. The change in reactivity is:

$$\rho = -\frac{\Delta\Sigma_t - \Delta\Sigma_s - \lambda\Delta(\nu\Sigma_f)}{\nu\Sigma_f + \Delta(\nu\Sigma_f)}. \tag{37}$$

Define the absorption cross section $\Sigma_a = \Sigma_t - \Sigma_s$ with corresponding change in the absorption cross section $\Delta\Sigma_a$ respectively. The analytic solution for $k_\infty$ of the perturbed system is:

$$k'_\infty = \frac{\nu\Sigma_f + \Delta(\nu\Sigma_f)}{\Sigma_a + \Delta\Sigma_a}. \tag{38}$$

The perturbation solution of $k$ is:

$$\tilde{k}'_\infty = -\frac{\nu\Sigma_f + \Delta(\nu\Sigma_f)}{\Sigma_a + \Delta\Sigma_a}. \tag{39}$$

Since both the analytic and perturbation are identical, $P/E$ is always unity for this simple problem.

***Two-Group Capture Cross Section Perturbation***

Suppose the capture cross sections are perturbed for the two-group problem used for the analytic $\Lambda$ solution. The removal cross section for group $g$ becomes: $\Sigma'_{Rg} = \Sigma_{Rg} + \Delta\Sigma_{cg}$. For simplicity, the unperturbed $k$ will be taken to be unity, although this is not necessary. From (10), it is possible to analytically determine $k'$:

$$k'_\infty = \frac{\nu\Sigma_{f1}\left(\Sigma_{R2} + \Delta\Sigma_{c2}\right) + \nu\Sigma_{f2}\Sigma_{s12}}{\left(\Sigma_{R1} + \Delta\Sigma_{c1}\right)\left(\Sigma_{R2} + \Delta\Sigma_{c2}\right)}. \tag{40}$$

Since the fission cross section is not perturbed, only the numerator of (34) changes:

$$\left\langle \psi^\dagger, \Delta\Sigma_c\psi \right\rangle = \frac{\Sigma_{R2}}{\nu\Sigma_{f2}}\Delta\Sigma_{c1} + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Delta\Sigma_{c2} \tag{41}$$

By combining this with the denominator from (15), the reactivity change is found:

$$\rho = -\frac{\frac{\Sigma_{R2}}{\nu\Sigma_{f2}}\Delta\Sigma_{c1} + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Delta\Sigma_{c2}}{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12}}. \tag{42}$$

The perturbed eigenvalue can be estimated fairly simply since $\lambda = 1$:

$$\tilde{k}'_\infty = \frac{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12}}{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12} + \frac{\Sigma_{R2}}{\nu\Sigma_{f2}}\Delta\Sigma_{c1} + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Delta\Sigma_{c2}}. \tag{43}$$

By taking the ratio of (43) and (40), it is possible to find $P/E$. Unlike with the previous problem, this is not, in general unity any longer. It is particularly instructive to consider the case where $\Delta\Sigma_{c1} = 0$ and $\Delta\Sigma_{c2}$ is positive and very large (for example, the introduction of a strong thermal absorber). The exact expression yields a return to the one-group solution in (4) since any scatter into group 2 is effectively lost from the system. The asymptotic limit of the perturbation solution, however, has the reactivity going to negative infinity, or a solution where no multiplication is possible.

### ***Two-Group Energy Transfer Cross Section Section Perturbation***

Suppose for the same problem as before, the scattering cross section of group 1 to 2, $\Sigma_{s12}$ is perturbed instead. There must also be a corresponding perturbation in the total cross section as well, $\Delta\Sigma_{t1} = \Delta\Sigma_{s12}$, so two terms are needed for the numerator. The analytic result for the perturbed $k_\infty$ is:

$$k'_\infty = \frac{\nu\Sigma_{f1}\Sigma_{R2} + \nu\Sigma_{f2}\left(\Sigma_{s12} + \Delta\Sigma_{s12}\right)}{\Sigma_{R2}\left(\Sigma_{R1} + \Delta\Sigma_{s12}\right)}. \tag{44}$$

The numerator of the reactivity expression is

$$\psi_1^\dagger \Delta\Sigma_{s12}\psi_1 + \psi_2^\dagger \Delta\Sigma_{s12}\psi_1 = \Delta\Sigma_{s12}\left(\frac{\Sigma_{R2}}{\nu\Sigma_{f2}} - 1\right). \tag{45}$$

Combining with the same denominator as last time, the reactivity can be expressed as

$$\rho = \frac{\Delta\Sigma_{s12}\left(1 - \frac{\Sigma_{R2}}{\nu\Sigma_{f2}}\right)}{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12}}. \tag{46}$$

Again, assuming the unperturbed case has $\lambda = 1$, the perturbed eigenvalue is

$$\tilde{k}'_\infty = \frac{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12}}{\frac{\nu\Sigma_{f1}}{\nu\Sigma_{f2}}\Sigma_{R2} + \Sigma_{s12} + \Delta\Sigma_{s12}\left(\frac{\Sigma_{R2}}{\nu\Sigma_{f2}} - 1\right)}. \tag{47}$$

This solution is particularly interesting because it can demonstrate how inaccurate perturbation theory may be. It is again useful to analyze the asymptotic behavior as $\Delta\Sigma_{s12}$ gets large. For the exact solution, all neutrons produced in group 1 almost immediately downscatter into group 2; no other reaction in group 1 matters. The value of $k_\infty$ in this case is the one-group solution using the group 2 cross sections.

Of particular interest for the perturbed solution is the case where $\Sigma_{R2}/\nu\Sigma_{f2} < 1$. In this case, the predicted eigenvalue will grow to infinity as it hits an asymptote and then promptly reaches an aphysical solution of a negative $k_\infty$ afterward.

### ***Two-Group $\nu$ Perturbation***

Suppose for the same problem, $\nu$ is increased separately for groups 1 and 2. The analytic solution for $k_\infty$ is:

$$k'_\infty = \frac{1}{\Sigma_{R1}}\left[\Sigma_{f1}\left(\nu_1 + \Delta\nu_1\right) + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Sigma_{f2}\left(\nu_2 + \Delta\nu_2\right)\right]. \tag{48}$$

This time, both the numerator and denominator of (34) must be considered. After manipulation (again, $\lambda = 1$), the change in reactivity is:

$$\rho = \frac{\Sigma_{f1}\Delta\nu_1 + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Sigma_{f2}\Delta\nu_2}{\Sigma_{f1}\left(\nu_1 + \Delta\nu_1\right) + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Sigma_{f2}\left(\nu_2 + \Delta\nu_2\right)}. \tag{49}$$

Correspondingly, the perturbed eigenvalue is:

$$\tilde{k}'_\infty = \frac{\Sigma_{f1}\left(\nu_1 + \Delta\nu_1\right) + \frac{\Sigma_{s12}}{\Sigma_{R2}}\Sigma_{f2}\left(\nu_2 + \Delta\nu_2\right)}{\nu_1\Sigma_{f1} + \frac{\Sigma_{s12}}{\Sigma_{R2}}\nu_2\Sigma_{f2}}. \tag{50}$$

Taking the ratio, $P/E$ is

$$P/E = \frac{\Sigma_{R1}}{\nu_1\Sigma_{f1} + \frac{\Sigma_{s12}}{\Sigma_{R2}}\nu_2\Sigma_{f2}} = \lambda = 1. \tag{51}$$

For this and similar problems, arbitrary increases in $\nu$ (even differing between energy groups) can be captured by perturbation theory perfectly. Note that this is no longer the case if $\lambda \neq 1$.

## 4 Summary

A set of analytic, infinite-medium problems has been developed for the point reactor kinetics parameters and reactivity perturbations using one or two energy groups. Given defined data, these solutions may be used to verify methods and implementations in simulation software. Also, the reactivity solutions may be used to compare the adjoint-weighted and differential operator methodologies of computing shifts in $k$. Further extensions would involve simple finite geometries such as 1-D slabs and spheres.