# 2-Group Diffusion Theory for Critical Systems

## Introduction

For the two-group approximation to multigroup diffusion theory,[1] one usually assumes no upscatter ($\Sigma_{2\to1} = 0$) and no fission source in group 2 ($\chi_1 = 1.0$ and $\chi_2 = 0.0$). With these specifications, the group 1 and 2 diffusion equations for a critical homogeneous system become

$$-D_1\nabla^2\phi_1 + \Sigma_{R1}\phi_1 - \lambda\left(\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2\right) = 0 \qquad (1)$$

$$-D_2\nabla^2\phi_2 + \Sigma_{a2}\phi_2 - \Sigma_{1\to2}\phi_1 = 0 \qquad (2)$$

where the 1 subscript refers to the fast group and the 2 represents the thermal group.

Solution of these equations for a general multidimensional, multi-region system is quite complicated (and beyond the scope of these notes). However, for the case of a 1-region bare homogeneous reactor, we can make a number of simplifying assumptions that lead to a system that is easy to solve and interpret. In particular, this procedure leads to formal expressions for $k_{eff}$ and the fast-to-thermal flux ratio in bare critical systems -- and, with the assumption of a large region, we get expressions for $k_\infty$ and $\phi_1/\phi_2$ for the particular material of interest. In the latter case, these neutronic material properties are very important in the design and analysis of thermal reactor systems.

## Bare Homogeneous Reactors

To develop the desired formulations we restrict our analysis to the case of a bare homogeneous 1-region critical system. In addition, we argue that the extrapolation distance in each energy group is the same (recall that $d \approx 2.13\ D$, so the extrapolation distance is really energy dependent). This latter approximation can be justified by the fact that the diffusion coefficient is not a strong function of energy, and that, in many cases, d is small compared to the reactor dimensions anyway. Thus, the minor variation of d with energy is usually negligible.

With the above assumption, we can argue that, for eqns. (1) and (2) to be valid at every point in the reactor, the spatial forms of $\phi_1(\vec{r})$ and $\phi_2(\vec{r})$ must be identical. This is easy to see in the case where the leakage term is small, since all the other terms simply have constant coefficients. However, from our study of 1-group theory, we also know that the flux curvature, $\nabla^2\phi$, is just proportional to the flux shape -- that is $\nabla^2\phi = -B^2\phi$, where $B^2$ is a constant. Thus, the spatial profile of the flux is indeed the same for each energy group, and the full solution to eqns. (1) and (2) can be written as

$$\phi_1(\vec{r}) = c_1\phi(\vec{r}) \qquad \text{and} \qquad \phi_2(\vec{r}) = c_2\phi(\vec{r}) \qquad (3)$$

where $\phi(\vec{r})$ satisfies an equation of the form

$$\nabla^2\phi(\vec{r}) + B^2\phi(\vec{r}) = 0 \qquad \text{or} \qquad \nabla^2\phi(\vec{r}) = -B^2\phi(\vec{r}) \qquad (4)$$

In these expressions, $\phi(\vec{r})$ (without a group subscript) represents only the spatial distribution of the flux, and $\phi_g(\vec{r}) = c_g\phi(\vec{r})$ (with a group subscript) represents the full space-energy solution. Note that this rationalization and the above summary mathematical relationships essentially

represent the assumption of space-energy separability in the system. In addition, since $\phi(\vec{r})$ represents the spatial profile from a 1-group bare system, we already know the distribution for all the common bare reactor geometries (see Refs. 2 - 4). Thus, once we specify the geometry, $\phi(\vec{r})$ is known and our challenge reduces to finding the discrete energy dependence of the flux (i.e. the $c_1$ and $c_2$ values).

Now, with the above separability assumption, substituting eqns. (3) and (4) into the matrix form of (1) and (2) gives

$$\begin{bmatrix} D_1B^2 + \Sigma_{R1} - \lambda\nu\Sigma_{f1} & -\lambda\nu\Sigma_{f2} \\ -\Sigma_{1\to2} & D_2B^2 + \Sigma_{a2} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{5}$$

where the flux distribution, $\phi(\vec{r})$, has canceled from the expression since we have a homogeneous system of equations.

The set of homogeneous algebraic equations will have a non-trivial solution if and only if the determinant of the coefficient matrix vanishes (i.e. the matrix must be singular). This is the ***criticality condition*** for the 2-group problem. Forcing the determinant of the 2×2 matrix to zero gives

$$\left(D_1B^2 + \Sigma_{R1} - \lambda\nu\Sigma_{f1}\right)\left(D_2B^2 + \Sigma_{a2}\right) - \lambda\nu\Sigma_{f2}\Sigma_{1\to2} = 0$$

and, separating out the terms containing the eigenvalue $\lambda$, gives

$$\left(D_1B^2 + \Sigma_{R1}\right)\left(D_2B^2 + \Sigma_{a2}\right) - \lambda\left[\nu\Sigma_{f1}\left(D_2B^2 + \Sigma_{a2}\right) + \nu\Sigma_{f2}\Sigma_{1\to2}\right] = 0$$

or
$$\lambda_n = \frac{\left(D_1B_n^2 + \Sigma_{R1}\right)\left(D_2B_n^2 + \Sigma_{a2}\right)}{\nu\Sigma_{f1}\left(D_2B_n^2 + \Sigma_{a2}\right) + \nu\Sigma_{f2}\Sigma_{1\to2}} \tag{6}$$

where the n subscript denotes that there are an infinite number of $B_n^2$'s that satisfy the critical bare reactor problem described by eqn. (4).[2-4]

Now, recalling that $\lambda = 1/k_{eff}$ for the fundamental mode (i.e. n = 1), we have

$$k_{eff} = \frac{\nu\Sigma_{f1}\left(D_2B^2 + \Sigma_{a2}\right) + \nu\Sigma_{f2}\Sigma_{1\to2}}{\left(D_1B^2 + \Sigma_{R1}\right)\left(D_2B^2 + \Sigma_{a2}\right)} \tag{7}$$

Recall also that the geometric buckling, $B^2$, is inversely proportional to the square of the characteristic dimension for the system of interest. Therefore, as the system becomes large, $B^2$ approaches zero. Thus, in the limit of an infinite system, we have

$$k_\infty = \frac{\nu\Sigma_{f1}\Sigma_{a2} + \nu\Sigma_{f2}\Sigma_{1\to2}}{\Sigma_{R1}\Sigma_{a2}} \tag{8}$$

where we note that this is a material property that characterizes the overall neutronic behavior [i.e. reactivity, $\rho_\infty = (k_\infty - 1)/k_\infty$] of the material -- a very important parameter indeed!

Also, from eqn. (3) we see that the two-group fluxes only differ by a constant, which is usually denoted by the fast-to-thermal flux ratio. From the matrix representation given in eqn. (5), we have

$$\frac{\phi_1}{\phi_2} = \frac{c_1}{c_2} = \frac{\lambda\nu\Sigma_{f2}}{D_1B^2 + \Sigma_{R1} - \lambda\nu\Sigma_{f1}} = \frac{D_2B^2 + \Sigma_{a2}}{\Sigma_{1\to 2}} \tag{9}$$

and for an infinite system this can be written as a simple ratio of cross sections, or

$$\left.\frac{\phi_1}{\phi_2}\right|_{\infty} = \frac{\Sigma_{a2}}{\Sigma_{1\to 2}} \tag{10}$$

This ratio is a good indicator of the general flux spectrum in a thermal system -- a somewhat softer spectrum will have a smaller $\phi_1/\phi_2$ value and a harder spectrum will have a larger fast-to-thermal flux ratio.

To complete this problem we need to normalize the spatial flux distribution to the reactor power

$$P = \kappa \sum_g \int \Sigma_{fg}(\vec{r})\phi_g(\vec{r})\,d\vec{r} \tag{11}$$

However, $\phi_g(\vec{r}) = c_g\phi(\vec{r})$ and, for a homogeneous system, the cross sections are spatially independent. Therefore, we can write the power as

$$P = \kappa\left(c_1\Sigma_{f1} + c_2\Sigma_{f2}\right)\int \phi\left(\vec{r}\right)d\vec{r} \tag{12}$$

Letting $c_2 = A$, we have

$$\phi_1(\vec{r}) = \frac{c_1}{c_2}A\phi(\vec{r}) = A\frac{\phi_1}{\phi_2}\phi(\vec{r}) \qquad \text{and} \qquad \phi_2(\vec{r}) = A\phi(\vec{r}) \tag{13}$$

Thus, the power expression becomes

$$P = \kappa\left[\Sigma_{f1}\frac{\phi_1}{\phi_2} + \Sigma_{f2}\right]A\int \phi\left(\vec{r}\right)d\vec{r} \tag{14}$$

or

$$A = \frac{P}{\kappa\left[\Sigma_{f1}\dfrac{\phi_1}{\phi_2} + \Sigma_{f2}\right]\displaystyle\int \phi\left(\vec{r}\right)d\vec{r}} \tag{15}$$

In these expressions, A is the overall flux normalization, $\phi_1/\phi_2$ is the fast-to-thermal flux ratio as given in eqn. (9), and the integral of the flux distribution has already been discussed for several simple reactor geometries (see Ref. 2 - 4).

This development is now complete. Although brief, there is a lot of meat here! We have seen that the flux shape in a 2-group model of a bare reactor is the same as the 1-group profile for each geometry of interest.[2-4] However, the expressions for the 2-group $k_{eff}$ and $k_\infty$ are quite different [see eqns. (7) and (8)] from their 1-group counterparts, since they take into account the production and loss of neutrons in both the fast and thermal groups. In addition, we introduced the fast-to-thermal flux ratio [eqn. (9)] and saw that this quantity is needed to define the fast flux,

and that it enters into consideration in the computation of the normalization. If the cross section data are available for a particular system, these expressions are relatively easy to use to compute critical size, critical composition, the value of $k_{eff}$ for a specific material-geometry combination, the maximum value of the flux for a given power level, etc. -- there is actually a lot of information that can be obtained here.

**The Four Factor Formula**

The above development of 2-group theory represents a formal treatment of this subject for bare systems. However, in many situations, the detailed cross section data needed to evaluate the above formal expressions are not readily available. The difficulty here often lies with determining the fast cross sections for the fuel (primarily $\Sigma_{f1}$ and $\Sigma_{a1}$ which are associated with fast fission and resonance absorption effects, respectively). Although these quantities can be computed accurately with sophisticated cross section processing codes, it would be nice to have an alternative, relatively simple approach for performing preliminary analyses. Towards this end, we will introduce the so-called ***four factor formula*** in this subsection and the basic ideas behind ***modified 1-group theory*** in the next subsection to give us some approximate 2-group computational capability without putting too much effort into generating formal values for $\Sigma_{f1}$ and $\Sigma_{a1}$.

In particular, let's focus on an infinite system for a moment. In such systems, of course, there is no leakage, so the only ultimate loss term is absorption. In the fast group, neutrons can get absorbed (primarily in the fuel and structure resonances) or scatter to thermal. At thermal, all the neutrons that have scattered from group 1 get absorbed, where some of the absorptions involve fission in the fuel. The fissions that occur (at both fast and thermal energies) produce neutrons at high energy, which starts the neutron life cycle all over again.

To describe this process in a quantitative manner, let's define a number of terms, as follows:

$$\text{thermal utilization} = f = \frac{\text{thermal absorption rate in fuel}}{\text{total thermal absorption rate}}$$

$$f = \frac{\int \Sigma_{a2}^{F}\phi_2 \, d\vec{r}}{\int \Sigma_{a2}\phi_2 \, d\vec{r}} = \frac{\overline{\Sigma}_{aF}\langle\phi_2\rangle}{\left(\overline{\Sigma}_{aF}+\overline{\Sigma}_{aM}\right)\langle\phi_2\rangle} = \frac{\overline{\Sigma}_{aF}}{\overline{\Sigma}_{aF}+\overline{\Sigma}_{aM}} = \frac{\overline{\Sigma}_{aF}}{\overline{\Sigma}_{a}} \qquad (16)$$

$$\text{reproduction factor} = \eta_T = \frac{\text{total neutrons emitted from thermal fission}}{\text{thermal neutrons absorbed in fuel}}$$

$$\eta_T = \frac{\int_T \eta(E)\Sigma_{aF}(E)\phi(E)dE}{\int_T \Sigma_{aF}(E)\phi(E)dE} = \frac{\langle \eta\Sigma_{aF}\phi\rangle_T}{\langle \Sigma_{aF}\phi\rangle_T}$$

or

$$\eta_T = \frac{\langle \nu\Sigma_f\phi\rangle_T}{\langle \Sigma_a^F\phi\rangle_T} = \frac{\nu\Sigma_{f2}}{\Sigma_{a2}^F}\frac{\langle\phi_2\rangle}{\langle\phi_2\rangle} = \frac{\nu\overline{\Sigma}_f}{\overline{\Sigma}_{aF}} \qquad (17)$$

$$\text{fast fission factor} = \varepsilon = \frac{\text{total neutrons emitted from all fission (fast and thermal)}}{\text{neutrons emitted from thermal fission}}$$

$$\varepsilon = \frac{\left\langle \nu\Sigma_{f1}\phi_1 \right\rangle + \left\langle \nu\Sigma_{f2}\phi_2 \right\rangle}{\left\langle \nu\Sigma_{f2}\phi_2 \right\rangle} = \frac{\nu\Sigma_{f1}\left\langle \phi_1/\phi_2 \right\rangle + \nu\Sigma_{f2}}{\nu\Sigma_{f2}} \tag{18}$$

resonance escape probability = p = probability that a fission neutron is not absorbed while slowing down

$$p = \frac{\left\langle \Sigma_{1\to2}\phi_1 \right\rangle}{\left\langle \Sigma_{a1}\phi_1 \right\rangle + \left\langle \Sigma_{1\to2}\phi_1 \right\rangle} = \frac{\Sigma_{1\to2}}{\Sigma_{a1} + \Sigma_{1\to2}} \tag{19}$$

To put these four terms to good use, let's define the thermal absorption rate as

$$\text{thermal absorption rate} = \int \Sigma_{a2}\phi_2 \, d\vec{r} = \Sigma_{a2}\left\langle \phi_2 \right\rangle = \overline{\Sigma}_a \left\langle \phi_2 \right\rangle = \left(\overline{\Sigma}_{aF} + \overline{\Sigma}_{aM}\right)\left\langle \phi_2 \right\rangle \tag{20}$$

where $\overline{\Sigma}_{aM}$ represents the absorption cross section in the moderator, coolant, structure, etc. (includes everything but fuel).

Now, we write several explicit expressions for the following quantities that describe the neutron life cycle:

1. number of thermal neutrons absorbed in reactor = $\overline{\Sigma}_a \left\langle \phi_2 \right\rangle = \overline{\Sigma}_a \left\langle \phi_T \right\rangle$
2. number of thermal neutrons absorbed in fuel = $f\,\overline{\Sigma}_a \left\langle \phi_T \right\rangle$
3. number of neutrons emitted from thermal fission = $\eta_T f\,\overline{\Sigma}_a \left\langle \phi_T \right\rangle$
4. number of neutrons emitted from all fission = $\varepsilon\,\eta_T f\,\overline{\Sigma}_a \left\langle \phi_T \right\rangle$
5. number of neutrons that make it to thermal in the next generation = $p\varepsilon\,\eta_T f\,\overline{\Sigma}_a \left\langle \phi_T \right\rangle$

Thus, we see that these terms can be used to help define the overall neutron balance in a 2-group infinite system. In particular, noting that the downscatter rate from group 1 to group 2, $\left\langle \Sigma_{1\to2}\phi_1 \right\rangle$, is equal to the thermal absorption rate, $\left\langle \Sigma_{a2}\phi_2 \right\rangle$, we can write an expression for the infinite multiplication factor as

$$k_\infty = \frac{\text{production rate}}{\text{loss rate}} = \frac{\varepsilon\,\eta_T f\,\overline{\Sigma}_a \left\langle \phi_T \right\rangle}{\Sigma_{a1}\left\langle \phi_1 \right\rangle + \overline{\Sigma}_a \left\langle \phi_T \right\rangle} = \frac{\varepsilon\,\eta_T f\,\overline{\Sigma}_a \left\langle \phi_T \right\rangle}{\Sigma_{a1}\left\langle \phi_1 \right\rangle + \Sigma_{1\to2}\left\langle \phi_1 \right\rangle} \tag{21}$$

But, from eqn. (19), we see that the denominator of this expression can be written in terms of the resonance escape probability as

$$\left\langle \Sigma_{a1}\phi_1 \right\rangle + \left\langle \Sigma_{1\to2}\phi_1 \right\rangle = \frac{\left\langle \Sigma_{1\to2}\phi_1 \right\rangle}{p}$$

Thus, the expression for $k_\infty$ is simply

$$k_\infty = \frac{\varepsilon\,\eta_T f\,p\overline{\Sigma}_a \left\langle \phi_T \right\rangle}{\Sigma_{1\to2}\left\langle \phi_1 \right\rangle} = \frac{\varepsilon\,\eta_T f\,p\overline{\Sigma}_a \left\langle \phi_T \right\rangle}{\overline{\Sigma}_a \left\langle \phi_T \right\rangle} = \eta_T f\,p\,\varepsilon \tag{22}$$

Thus, the so-called ***four factor formula*** is just a simple expression for the multiplication factor in an infinite system, $k_\infty = \eta_T f\, p\, \varepsilon$. This is an important result -- $k_\infty$ is a material property that characterizes the reactivity potential of a particular material composition.

It is also very instructive to show that our two expressions for $k_\infty$ are identical [that is, that eqn. (8) and eqn. (22) give the same value]. To show this, we expand the expression for $k_\infty = \eta_T f\, p\, \varepsilon$ in terms of the four factors written in full detail, or

$$k_\infty = \left[\frac{\langle \nu\Sigma_{f2}\phi_2\rangle}{\langle \Sigma_{a2}^F\phi_2\rangle}\right]\left[\frac{\langle \Sigma_{a2}^F\phi_2\rangle}{\langle \Sigma_{a2}\phi_2\rangle}\right]\left[\frac{\langle \Sigma_{1\to2}\phi_1\rangle}{\langle \Sigma_{R1}\phi_1\rangle}\right]\left[\frac{\langle \nu\Sigma_{f1}\phi_1\rangle + \langle \nu\Sigma_{f2}\phi_2\rangle}{\langle \nu\Sigma_{f2}\phi_2\rangle}\right]$$

and, cancelling the factors contained in both the numerator and denominator, gives

$$k_\infty = \left[\frac{\langle \nu\Sigma_{f1}\phi_1\rangle + \langle \nu\Sigma_{f2}\phi_2\rangle}{\langle \Sigma_{a2}\phi_2\rangle}\right]\left[\frac{\langle \Sigma_{1\to2}\phi_1\rangle}{\langle \Sigma_{R1}\phi_1\rangle}\right]$$

But, we have already noted that, in an infinite system, the downscatter rate from the fast group, $\langle \Sigma_{1\to2}\phi_1\rangle$, is equal to the thermal absorption rate, $\langle \Sigma_{a2}\phi_2\rangle$. Thus, the above expression reduces to

$$k_\infty = \frac{\langle \nu\Sigma_{f1}\phi_1\rangle + \langle \nu\Sigma_{f2}\phi_2\rangle}{\langle \Sigma_{R1}\phi_1\rangle} = \frac{\nu\Sigma_{f1}(\phi_1/\phi_2) + \nu\Sigma_{f2}}{\Sigma_{R1}(\phi_1/\phi_2)} = \frac{\nu\Sigma_{f1}(\Sigma_{a2}/\Sigma_{1\to2}) + \nu\Sigma_{f2}}{\Sigma_{R1}(\Sigma_{a2}/\Sigma_{1\to2})}$$

or $$k_\infty = \frac{\nu\Sigma_{f1}\Sigma_{a2} + \nu\Sigma_{f2}\Sigma_{1\to2}}{\Sigma_{R1}\Sigma_{a2}}$$

where we have used the expression for the fast-to-thermal flux ratio in an infinite system from eqn. (10) in the last manipulation step. This last expression is identical to the formal statement given in eqn. (8).

Therefore, with the proper definition of the individual terms, the four factor formula is identical to the expression derived from formal 2-group theory for infinite homogeneous systems. Either expression for the 2-group $k_\infty$ can be used as desired, where

$$k_\infty = \frac{\nu\Sigma_{f1}\Sigma_{a2} + \nu\Sigma_{f2}\Sigma_{1\to2}}{(\Sigma_{a1} + \Sigma_{1\to2})\Sigma_{a2}} \qquad \text{or} \qquad k_\infty = \eta_T f\, p\, \varepsilon$$

**The Six Factor Formula and Modified 1-Group Theory**

Using the terms from the four factor formula to rewrite the 2-group diffusion model slightly, we can also develop an alternate expression for $k_{eff}$. To do this we will follow the procedure from Lamarsh.[4] In particular, we start with the formal 2-group neutron balance equation given in eqns. (1) and (2), with the following changes/assumptions:

1. Rewrite the fission source term as

$$S^{fission} = \lambda(\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2) = \lambda\varepsilon\eta_T f\,\Sigma_{a2}\phi_2 = \lambda\frac{k_\infty}{p}\Sigma_{a2}\phi_2 \qquad \text{(no approximations here)}$$

2. Make the assumption that the fast absorption cross section is small compared to the downscatter cross section, or

$$\Sigma_{R1} = \Sigma_{a1} + \Sigma_{1\to 2} \approx \Sigma_{1\to 2} \qquad \text{(assumes } \Sigma_{a1} << \Sigma_{1\to 2}\text{)}$$

3. Modify the downscatter source to account for the above assumption -- since the fast flux will be somewhat high due to the elimination of the fast absorption term, we reduce the downscatter rate by the resonance escape probability, or

$$S^{\text{downscatter}} = \Sigma_{1\to 2}\phi_1 \Rightarrow p\Sigma_{1\to 2}\phi_1 \qquad \text{(tries to correct for setting } \Sigma_{a1}\phi_1 = 0\text{)}$$

With these modifications, the fast and thermal balance equations become

$$-D_1\nabla^2\phi_1 + \Sigma_{1\to 2}\phi_1 - \lambda\frac{k_\infty}{p}\Sigma_{a2}\phi_2 = 0 \tag{23}$$

$$-D_2\nabla^2\phi_2 + \Sigma_{a2}\phi_2 - p\Sigma_{1\to 2}\phi_1 = 0 \tag{24}$$

Now, using eqns. (23) and (24), we can follow the same procedure as before to derive an expression for $k_{eff}$ for the system of interest. Again we let $\phi_g(\vec{r}) = c_g\phi(\vec{r})$ where the spatial solution is given by an equation of the form $\nabla^2\phi + B^2\phi = 0$ (i.e. the 1-group critical reactor equation). Then, upon substitution and putting the resultant algebraic equations into matrix form, we have

$$\begin{bmatrix} D_1B^2 + \Sigma_{1\to 2} & -\lambda\dfrac{k_\infty}{p}\Sigma_{a2} \\ -p\Sigma_{1\to 2} & D_2B^2 + \Sigma_{a2} \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{25}$$

Again the determinant of the coefficient matrix must be zero for a non-trivial solution, or

$$\left(D_1B^2 + \Sigma_{1\to 2}\right)\left(D_2B^2 + \Sigma_{a2}\right) - \lambda k_\infty\Sigma_{1\to 2}\Sigma_{a2} = 0$$

and solving for $\lambda$ gives

$$\lambda = \frac{\left(D_1B^2 + \Sigma_{1\to 2}\right)\left(D_2B^2 + \Sigma_{a2}\right)}{k_\infty\Sigma_{1\to 2}\Sigma_{a2}}$$

or

$$k_{eff} = \frac{1}{\lambda} = \frac{k_\infty\Sigma_{1\to 2}\Sigma_{a2}}{\left(D_1B^2 + \Sigma_{1\to 2}\right)\left(D_2B^2 + \Sigma_{a2}\right)} \tag{26}$$

This expression should be compared to that given in eqn. (7) -- which was derived from formal 2-group theory with minimal approximations. Equation (26), on the other hand, has several additional assumptions and, therefore, it is only an approximation to the result given by eqn. (7). However, for preliminary estimates of $k_{eff}$, eqn. (26) is often much easier to apply because a formal set of 2-group macroscopic cross sections are not required. To see this more clearly, recall the definitions of the thermal neutron age, $\tau_T$, and thermal diffusion area, $L_T^2$, where

$$\tau_T = \frac{D_1}{\Sigma_{1\to 2}} \qquad \text{and} \qquad L_T^2 = \frac{D_2}{\Sigma_{a2}}$$

Using these definitions, we see that division of the numerator and denominator of eqn. (26) by $\Sigma_{1\to 2}\Sigma_{a2}$ directly leads to

$$k_{eff} = k_\infty \left( \frac{1}{1+\tau_T B^2} \right) \left( \frac{1}{1+L_T^2 B^2} \right) \tag{27}$$

where the two factors in parentheses are formal expressions for the fast and thermal non-leakage probabilities in the system. In particular, for the fast group, neutrons can either leak out of the system or downscatter to the thermal group (recall we are assuming that $\Sigma_{a1} << \Sigma_{1\to 2}$). Thus, the fast non-leakage probability (or fast removal probability) is given by

$$P_F = \frac{\langle \Sigma_{1\to 2}\phi_1 \rangle}{\langle D_1 B^2 \phi_1 \rangle + \langle \Sigma_{1\to 2}\phi_1 \rangle} = \frac{1}{1+\tau_T B^2} \tag{28}$$

Using similar arguments for the thermal group leads to an expression for the thermal non-leakage probability, or

$$P_T = \frac{\langle \Sigma_{a2}\phi_2 \rangle}{\langle D_2 B^2 \phi_2 \rangle + \langle \Sigma_{a2}\phi_2 \rangle} = \frac{1}{1+L_T^2 B^2} \tag{29}$$

Thus, with these definitions, the expression for the multiplication factor in a bare homogeneous reactor can be written as

$$k_{eff} = k_\infty P_T P_F \tag{30}$$

Since $k_\infty = \eta_T f p \varepsilon$ (i.e. the 4-factor formula), the expression for $k_{eff}$ in eqn. (30) is often called the **six factor formula** -- that is $k_{eff} = \eta_T f p \varepsilon P_F P_T$ -- and it is often easier to estimate the terms within this expression than to determine the formal 2-group macroscopic cross sections needed for eqn. (7). Thus, the 6-factor formula is quite important when performing preliminary computations of critical size or critical composition, and it is also quite useful in describing the life cycle of neutrons in a thermal reactor.

Within the life-cycle context, Fig. 1 gives a specific example that illustrates how the elements of the 6-factor formula can be used to identify the neutron population at several stages within its life cycle. Note that numerical values for the six factors are given that lead to $k_{eff}$ = 1.000 (see Fig. 1 for the specific values). The demo starts with 1000 neutrons that are born from thermal fission (this is $N_o$ in the sketch). This neutron population is increased by a factor of $\varepsilon$ to account for the fast fissions that can occur. These fast neutrons, $N_o\varepsilon$, can either leak out of the finite system, be absorbed as fast neutrons, or scatter down to the thermal group. Since $P_F$ gives the fast non-leakage probability, and p gives the resonance escape probability, then $(N_o\varepsilon)P_F p$, gives the number of neutrons that do indeed downscatter to thermal energies.

At thermal, the neutrons can either leak out of the system or be absorbed, with a fraction of the absorptions taking place in the fuel material. Since $P_T$ is the thermal non-leakage probability and f is the fraction of absorptions that take place in the fuel, then $(N_o\varepsilon P_F p)P_T f$ thermal neutrons

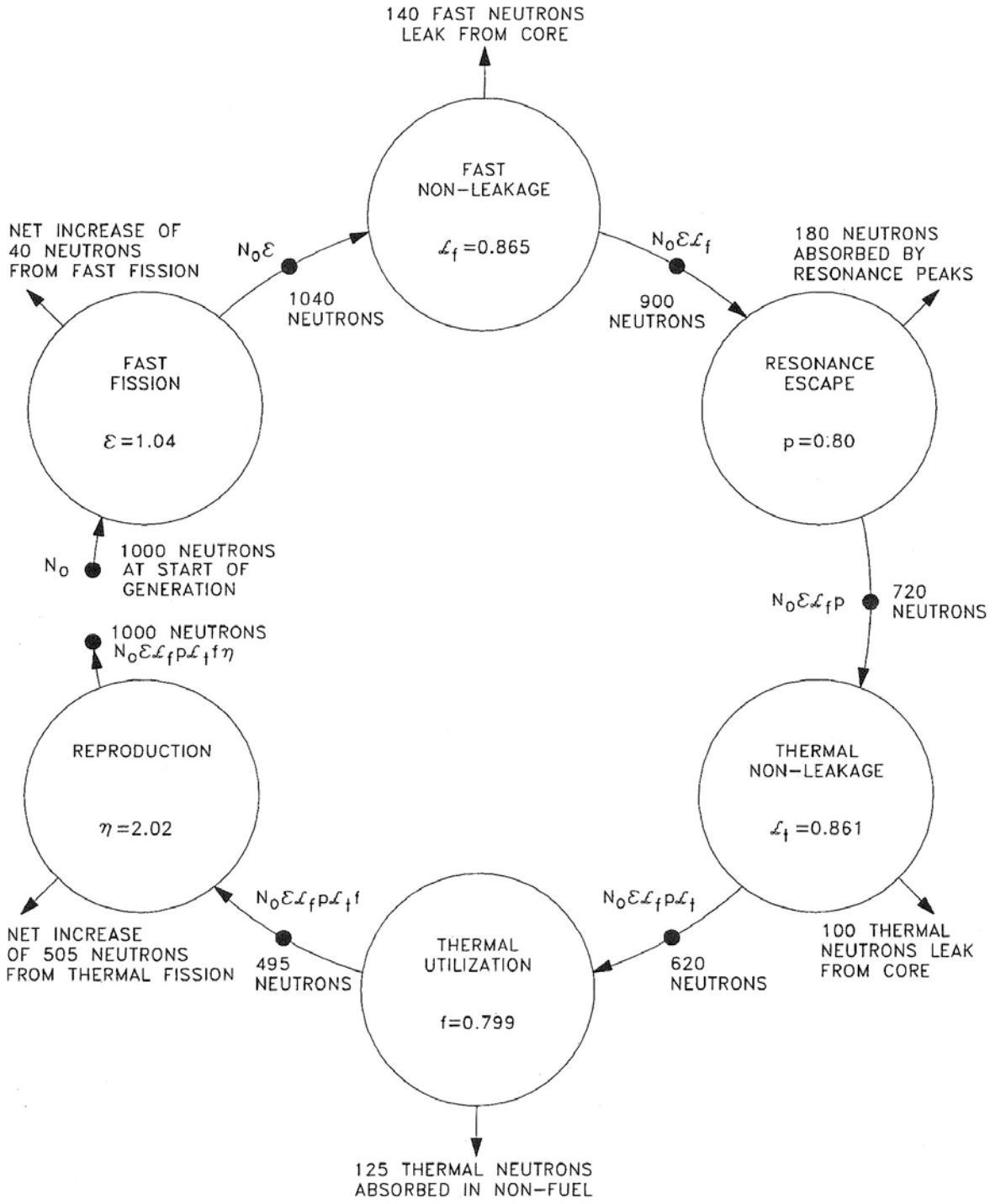


**Fig. 1 Neutron life cycle with $k_{eff}$ = 1.000 (directly from Ref. 5).**

actually get absorbed in the fuel material. Finally, since $\eta_T$ gives the neutrons emitted from thermal absorption in the fuel, then $(N_o \varepsilon P_F p P_T f)\eta_T$ fission neutrons will be produced in the next generation from thermal fission -- and since $k_{eff} = \eta_T f p \varepsilon P_F P_T = \eta_T f p \varepsilon L_F L_T = 1.000$ in this example, then the original number of $N_o$ neutrons are emitted from thermal fission to start a new life cycle (note that Fig. 1 uses $L_F$ and $L_T$ to denote the fast and thermal non-leakage probabilities and we have been using $P_F$ and $P_T$ for these quantities -- clearly these are equivalent terms, where $L_F = P_F$ and $L_T = P_T$).

Now, as a final task for this subsection, we will also put eqn. (27) or (30) into a form similar to 1-group theory -- that is, we want to develop the so-called **modified 1-group formula** for $k_{eff}$. First we recall the 1-group expressions (see Ref. 2),

$$k_{eff} = \frac{k_\infty}{1 + L^2 B^2} = k_\infty P_{NL} \tag{31}$$

where $P_{NL}$ is the non-leakage probability and $k_\infty = \eta f$ (note that $k_\infty = \eta f$ is sometimes referred to as the 2-factor formula and $k_{eff} = k_\infty P_{NL} = \eta f P_{NL}$ is often called the 3-factor formula -- both these are associated with the 1-group approximation).

Getting back to the 2-group problem, let's expand the denominator of the criticality condition given in eqn. (27),

$$k_{eff} = \frac{k_\infty}{\left(1 + L_T^2 B^2\right)\left(1 + \tau_T B^2\right)} = \frac{k_\infty}{1 + \left(L_T^2 + \tau_T\right) B^2 + L_T^2 \tau_T B^4}$$

For a large system, $B^2$ is quite small and $B^4$ is very small. In this case, the following inequality is often valid

$$L_T^2 \tau_T B^4 << \left(L_T^2 + \tau_T\right) B^2$$

and we can write the following "modified 1-group theory" critical condition as

$$k_{eff} = \frac{k_\infty}{1 + \left(L_T^2 + \tau_T\right) B^2} = \frac{k_\infty}{1 + M_T^2 B^2} \tag{32}$$

where $M_T^2 = L_T^2 + \tau_T$ is the thermal migration area.

Equation (32) is the desired expression for so-called **modified 1-group theory**. It is an estimate of the multiplication factor for the 2-group approximation to multigroup diffusion theory in bare homogeneous systems. Note, however, that this expression looks very similar to the 1-group representation given in eqn. (31) and it is used in a similar manner. Thus, eqn. (32) is called the "modified" 1-group formula simply because it resembles the 1-group expression -- however, always remember that it is associated with 2-group theory.

**Critical Size and Critical Composition Calculations (for dilute homogeneous systems)**

The above development is used in preliminary computations for the critical size and critical composition of simple homogeneous bare core configurations. In addition, the same basic techniques can also be used for reflected cores, if some information about the reflector savings, $\delta$, is known. The hand computations rely on a number of assumptions that allow one to readily

estimate the parameters within the modified 1-group theory expression for $k_{eff}$ as given in eqn. (32). In particular, the assumption of a **dilute homogeneous system** is key to resolving a lot of the necessary data for the calculations -- where the word "dilute" implies that the fuel composition is only a small component of the overall homogeneous mixture.

For example, for a two-component dilute homogeneous system (consisting of only fuel and moderator -- where the "moderator" here is everything but fuel), the macroscopic cross sections for the mixture can be approximated as follows:

The ***transport cross section*** is given as

$$\Sigma_{tr} = \Sigma_{tr}^{F} + \Sigma_{tr}^{M} = N^{F}\sigma_{tr}^{F} + N^{M}\sigma_{tr}^{M}$$

But, although the microscopic data are on the same order of magnitude (i.e. $\sigma_{tr}^{F}$ is of the same order as $\sigma_{tr}^{M}$), the dilute nature of the mixture tells us that $N^{M} >> N^{F}$. Because of this condition, the expression for the transport cross section reduces to

$$\Sigma_{tr} \approx N^{M}\sigma_{tr}^{M} \approx \Sigma_{tr}^{M}$$

and the ***diffusion coefficient*** for the mixture becomes

$$D = \frac{1}{3\Sigma_{tr}} \approx \frac{1}{3\Sigma_{tr}^{M}} = D_{M} \qquad (33)$$

Thus, the diffusion coefficient of the moderator can usually be used to approximate the diffusion coefficient for the overall mixture.

Similarly, for the ***downscatter cross section***, we make the same set of assumptions, giving

$$\Sigma_{1\to 2} = \Sigma_{1\to 2}^{F} + \Sigma_{1\to 2}^{M} \approx \Sigma_{1\to 2}^{M} \qquad (34)$$

and with the approximations in eqns. (33) and (34), we can write the ***thermal neutron age*** as

$$\tau_{T} = \frac{D_{1}}{\Sigma_{1\to 2}} \approx \frac{D_{1}^{M}}{\Sigma_{1\to 2}^{M}} \qquad \text{or} \qquad \tau_{T} = \tau_{TM} \qquad (35)$$

For a homogeneous system, the basic definition of the ***thermal utilization*** gives

$$f = \frac{\overline{\Sigma}_{a}^{F}}{\overline{\Sigma}_{a}} = \frac{\overline{\Sigma}_{a}^{F}}{\overline{\Sigma}_{a}^{F} + \overline{\Sigma}_{a}^{M}} = \frac{\overline{\Sigma}_{a}^{F}/\overline{\Sigma}_{a}^{M}}{\overline{\Sigma}_{a}^{F}/\overline{\Sigma}_{a}^{M} + 1} = \frac{z}{z+1} \qquad (36)$$

where we have defined $z = \overline{\Sigma}_{a}^{F}/\overline{\Sigma}_{a}^{M}$ as the ratio of the fuel and moderator thermal absorption cross sections (this is done simply for convenience in subsequent manipulations).

With this definition of f, we can write an expression for the ***thermal diffusion area*** as

$$L_{T}^{2} = \frac{D_{2}}{\Sigma_{a2}} \approx \frac{\overline{D}_{M}}{\overline{\Sigma}_{a}} = \frac{\overline{D}_{M}}{\overline{\Sigma}_{a}^{F} + \overline{\Sigma}_{a}^{M}} = \frac{\overline{D}_{M}/\overline{\Sigma}_{a}^{M}}{\overline{\Sigma}_{a}^{F}/\overline{\Sigma}_{a}^{M} + 1} = \frac{L_{TM}^{2}}{z+1}$$

and, noting that

$$1-f=1-\frac{z}{z+1}=\frac{1}{z+1}$$

we have

$$L_T^2=(1-f)L_{TM}^2 \tag{37}$$

Note that, if the temperature or the moderator density are different from nominal conditions (i.e. 20 $^oC$ and nominal density), then all the cross sections used in the above expressions need to be temperature and density corrected, as appropriate. The reader should see Refs. 4 or 6 for further information on this "correction" procedure.

One final, but very important assumption, concerns the ***resonance escape probability*** and the ***fast fission factor***. In dilute homogeneous systems, the resonance escape probability, p, is slightly less than unity and the fast fission factor, ε, is slightly greater than unity. However, beyond these simple qualitative statements, it is not easy to get a good quantitative estimate for either of these quantities (not without a fair amount of effort). Thus, in preliminary calculations, it is often assumed that the product of these two factors is approximately unity, or

$$p\varepsilon \approx 1.0 \quad \text{(for dilute homogeneous systems)} \tag{38}$$

Now, with some background on the various approximations involved and the above expressions for several of the needed intermediate quantities, we are ready to outline the actual computations required in typical analyses. In particular, the problem solution scheme is somewhat different for the two cases of interest here, as follows:

### *1. Given the Material Composition, Compute the Critical Size*

This is the easier of the two cases. Here, with the fuel and moderator compositions known, one can obtain cross section data for the fuel and moderator (from the various data tables in Ref. 4 or from the **cross_sections_gui** program as discussed in Ref. 6, for example) and compute the values of $k_\infty \approx \eta f$ and $M_T^2 = L_T^2 + \tau_T$. Then, setting $k_{eff} = 1$ for the critical case, we can solve eqn. (32) for the buckling,

$$B^2=\frac{k_\infty-1}{M_T^2} \tag{39}$$

and compute the desired critical dimension -- recall that the core size and geometric buckling are simply related for each of the simple core geometries often treated in preliminary computations (see Refs. 2 - 4, for example).

### *2. Given the Core Size, Compute the Critical Fuel Composition*

For this case, we can immediately compute the buckling from the known core dimensions. However, since we don't know the fuel composition, $N^F$, or $N^F\bar{\sigma}_a^F$, or $z=\bar{\Sigma}_a^F/\bar{\Sigma}_a^M$, we simply write the expression for $k_{eff}$ in terms of one of these quantities, and then solve for this unknown quantity (the expression for z is often used for convenience).

Thus, using eqns. (36) and (37) within eqn. (32) for the critical case gives

$$k_{eff} = 1 = \frac{\eta_T z/(z+1)}{1 + B^2\left(\frac{L_{TM}^2}{z+1} + \tau_{TM}\right)} \tag{40}$$

Now we simply solve this expression for z in terms of the material properties $\eta_T$, $L_{TM}^2$, and $\tau_{TM}$ and the geometric buckling, $B^2$. Doing the algebra gives

$$1 = \frac{\frac{\eta_T z}{z+1}}{1 + B^2\left(\frac{L_{TM}^2}{z+1} + \tau_{TM}\frac{z+1}{z+1}\right)} = \frac{\frac{\eta_T z}{z+1}}{\frac{z+1+B^2L_{TM}^2 + B^2\tau_{TM}(z+1)}{z+1}}$$

$$1 = \frac{\eta_T z}{z + B^2\tau_{TM}z + 1 + B^2L_{TM}^2 + B^2\tau_{TM}}$$

$$\eta_T z = z\left(1 + B^2\tau_{TM}\right) + 1 + B^2\left(L_{TM}^2 + \tau_{TM}\right)$$

$$\left[\eta_T - \left(1 + B^2\tau_{TM}\right)\right]z = 1 + B^2\left(L_{TM}^2 + \tau_{TM}\right)$$

and finally we get

$$z = \frac{1 + B^2\left(L_{TM}^2 + \tau_{TM}\right)}{\eta_T - 1 - B^2\tau_{TM}} \tag{41}$$

This expression is used for simple hand computations when the geometry is known (i.e. $B^2$ is known) and one needs to compute the critical composition (i.e. for $k_{eff} = 1.000$). Once z has been determined via eqn. (41), then

$$\bar{\Sigma}_a^F = z\,\bar{\Sigma}_a^M \qquad \text{and} \qquad N_F = z\,N_M\frac{\bar{\sigma}_a^M}{\bar{\sigma}_a^F} \tag{42}$$

which is the usual desired result from a "critical composition calculation."

**The diluteh_gui Code**

The methodology described in the previous subsection is based on the approach used in Lamarsh (Ref. 4). An easier, and possibly more useful technique would be to simply compute $k_{eff}$ for the given geometry and material combination. One can, for example, compute $k_{eff}$ directly for each combination of fuel composition (i.e. known z or f) and core size (i.e. known $B^2$). With this ability, one can easily perform a parametric study for any parameter of interest. For the Case 1 scenario, one holds the composition fixed and varies the core size, each time computing $k_{eff}$ for the given core size. Then, a simple plot of $k_{eff}$ vs. core size will easily show the critical core size (i.e. when $k_{eff} = 1.000$) as well as show how rapidly the multiplication factor changes with the core dimensions. Similarly, for the Case 2 situation, one holds the core size fixed and varies the fuel composition -- again leading to information on how $k_{eff}$ varies with the fuel loading as well as the specific critical fuel composition. This approach is actually more intuitive (i.e. performing a simple parametric study) and it bypasses the intermediate steps and algebra that lead to

eqn. (41). Instead, one simply puts the computed values of $B^2$, $k_\infty \approx \eta f$, and $M_T^2 = L_T^2 + \tau_T$ into the modified 1-group formula in eqn. (32) and computes $k_{eff}$ directly for the given geometry and materials combination -- this is a much more straightforward approach to the problem.

This more direct parametric approach has been implemented into the **diluteh_gui** code. This Matlab program simply provides a user-friendly interface for performing the modified 1-group theory computations identified in this set of Lecture Notes. The code is set up to handle both bare and reflected systems (see below) and to allow a variety of core geometries and material compositions. The cross sections needed for the calculations are built into the code and the user interface, as shown in Fig. 2, is similar in construction to the **cross_sections_gui** code discussed previously (see Ref. 6). Of course, the **diluteh_gui** code also allows the user to specify the geometry parameters as well as the material composition. In addition, the code automatically varies the core dimensions and produces a parametric plot of $k_{eff}$ vs. core size, as illustrated in Fig. 3. Finally, we note that a data file containing many of the intermediate results of the overall calculation is available via the ***Save Data/Results*** button in the center of the GUI window. For reference, a sample data file corresponding to the case illustrated in Figs. 2 and 3 is included in Table 1. This type of information can be very useful for checking hand calculations and for gaining a good understanding of exactly what the code is doing.

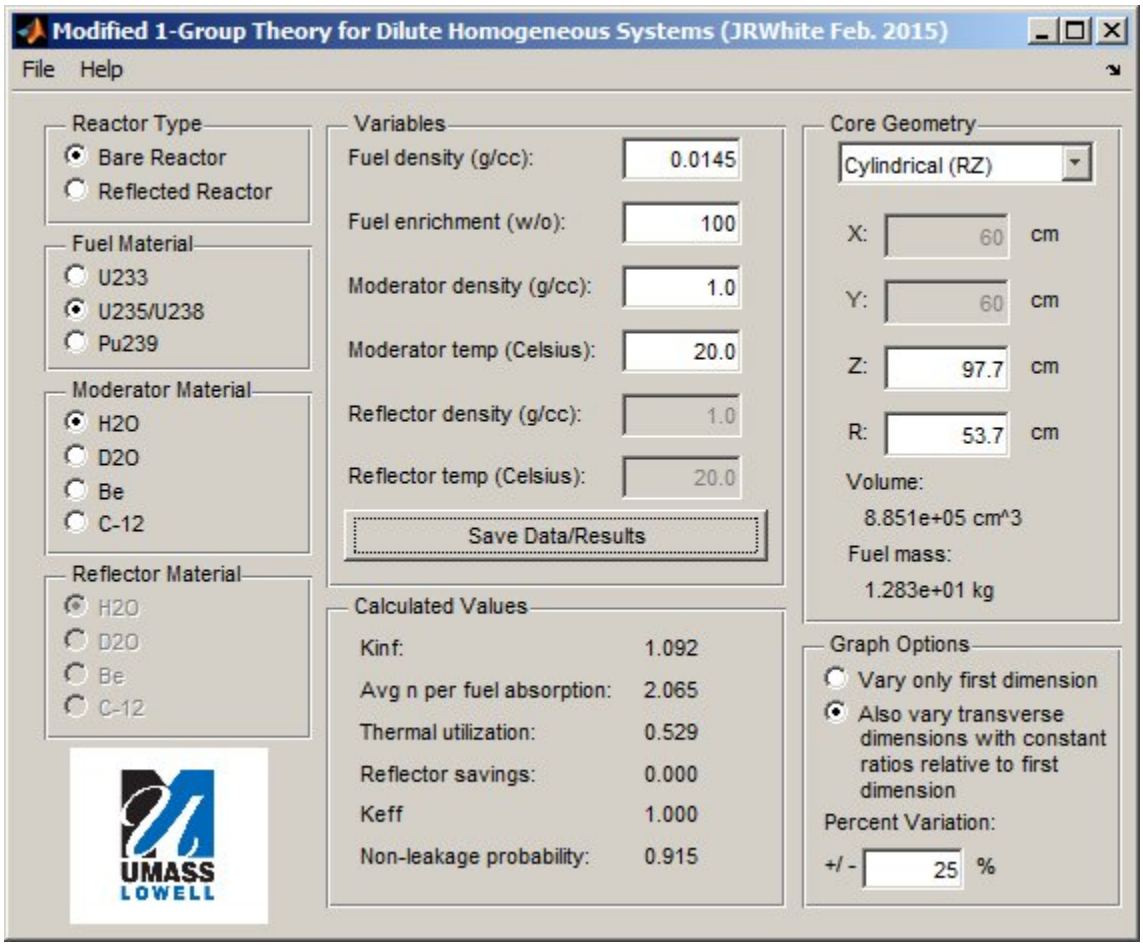


**Fig. 2 The diluteh_gui interface.**

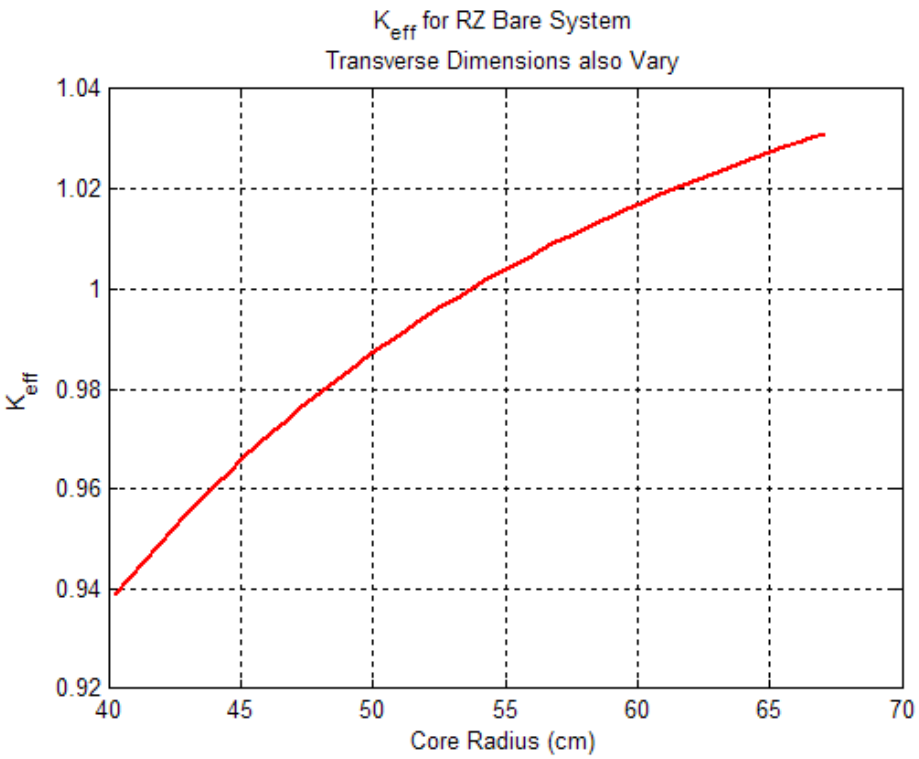


**Fig. 3 Parametric study for $k_{eff}$ vs. core size.**

**Table 1 Sample data file from the diluteh_gui code.**

```
    Computation of Kinf for a dilute homogeneous   Bare Reactor

Material Description for Problem
  Fuel Material:                    U235/U238
  Fuel Density (g/cc):               1.450e-002
  Fissile Enrichment (w/o):         100.000
  Moderator Material:               H20
  Moderator Density (g/cc):          1.000
  Temperature of fuel/mod mix (C): 20.000

Calculated Parameters for Kinf
  kinf =  1.092
  eta  =  2.065
  f    =  0.529
  pe   =  1.000

Some Additional Material Data
  Sffiss (1/cm) =    1.886e-002
  Safiss (1/cm) =    2.212e-002
  Safert (1/cm) =    0.000e+000
  SaF    (1/cm) =    2.212e-002
  SaM    (1/cm) =    1.970e-002
  DM     (cm)   =    1.600e-001
  LT2M   (cm^2) =    8.122e+000
  TAUM   (cm^2) =    2.697e+001
```

```
  MT2    (cm^2) =    3.079e+001
  DR     (cm)   =    0.000e+000
  LT2R   (cm^2) =    0.000e+000


    Computation of Keff for above   Bare Reactor    System


System Description
  Geometry Type:          Cylindrical Geometry (RZ)
  Core Dimensions (cm):   53.70 97.70
  Core Vol (cc):           8.851e+005
  Fuel Mass (kg):          1.283e+001
  Reflector Savings (cm):  0.000e+000
  Buckling (1/cm^2):       3.000e-003

Calculated Parameters
  Non-Leakage Probability:  0.915
  Keff:                     1.000
```

Overall, the **diluteh_gui** code is easy to use and it saves considerable time and effort when analyses of this type are needed -- and the reader is certainly encouraged to give it a try…

**Reflected Core Calculations**

As a final note, we should emphasize that the above computations are only directly applicable for the solution of bare homogeneous critical core problems, since the modified 1-group formula for $k_{eff}$ was derived explicitly for this situation. However, Ref. 4 discusses how to view a core-reflector system as a bare core with an effective core size that is increased to account for the effect of the reflector on the system. In particular, the reflector savings, $\delta$, is defined as the difference in the critical dimension of the bare and reflected systems. Clearly, since the reflector reduces the net leakage, the critical size of a reflected core will be smaller than the size of a bare critical core. Or, from a different perspective, if a bare core with a given $k_{eff}$ is surrounded by an infinite reflector, then the system multiplication factor will increase.

With the above simple rationalization, one can estimate $k_{eff}$ for the reflected system by simply increasing the physical core size by the reflector savings and then use the above methodology for a hypothetical bare core with the increased "effective core size". In particular, Lamarsh (Ref. 4) gives approximate correlations for estimating the reflector savings in thermal systems, where

$$\delta \approx \frac{\overline{D}_c}{\overline{D}_r} L_{Tr} \qquad \text{(for all but water systems)} \tag{43}$$

and

$$\delta \approx 7.2 + 0.10\left(M_T^2 - 40.0\right) \qquad \text{(for water moderated and reflected systems)} \tag{44}$$

With a known $\delta$, the effective buckling for a reflected parallelepiped reactor, for example, becomes

$$B^2 = \left(\frac{\pi}{a+2\delta}\right)^2 + \left(\frac{\pi}{b+2\delta}\right)^2 + \left(\frac{\pi}{c+2\delta}\right)^2 \tag{45}$$

where a, b, and c are the real core dimensions, and a + 2δ, b + 2δ, and c + 2δ are the effective dimensions used to account for the reduced leakage that will occur in the reflected system. With this simple change, the above modified 1-group methodology for bare cores can also be easily applied to reflected systems.

This simple "effective core size" approach for reflected systems has been implemented into the **diluteh_gui** code so that approximate critical size and composition calculations can be made for both bare and reflected systems…

**Summary**

This set of Lecture Notes has developed a set of formal expressions for performing 2-group analytical computations for bare and reflected core configurations. Several variants, including formal 2-group theory, the 4-factor and 6-factor formulas, and a more approximate modified 1-group theory formulation, have been developed and discussed, and the reader should now have a better understanding of this methodology and its application for computing the critical size and composition of thermal reactor systems. These techniques are actually quite useful for obtaining preliminary estimates of various criticality parameters, and the terminology and insight gained here are essential tools for understanding and interpreting more complicated systems -- and the **diluteh_gui** code makes it really easy to actually do these types of analyses. Overall, the background gained here will definitely be useful in the future, and it makes a significant addition to your fundamental knowledge and understanding of basic reactor theory -- since the concepts introduced here will indeed be useful in the core design process, in reload design analyses, in discussing reactor operations, etc., etc…

**References**


1. J. R. White, "The Multigroup Neutron Balance Equation," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.
2. J. R. White, "1-D Bare and Reflected Critical Systems Using 1-Group Diffusion Theory," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell. This set of Lecture Notes also provides documentation for the ***core_refl1g_gui*** Matlab program.
3. J. R. White, "The Bare Critical Finite Cylindrical Reactor," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell.
4. J. R. Lamarsh and A. J. Baratta, ***Introduction to Nuclear Engineering***, 3rd Edition, Prentice Hall (2001).
5. ***DOE Fundamentals Handbook: Nuclear Physics and Reactor Theory (Vol 2)***, DOE-HDBK-1019/2-1993.
6. J. R. White, "Cross Section Data for Preliminary Calculations," part of a series of Lecture Notes for the Nuclear Engineering Program at UMass-Lowell. This set of Lecture Notes also provides documentation for the ***cross_sections_gui*** Matlab program.