## INTRODUCTION

The objective of distributing materials in a nuclear system, multiplying or fixed-source, is to maximize (or minimize) some quantity of interest such as minimizing the fissile mass in a nuclear fission reactor, maximizing the tritium production in a fusion blanket, or minimizing the radiation environment surrounding a detection system. Thus, optimal distributions lie at the heart of design optimization for which variational methods [1-5] are extensively used although often for idealized configurations. Further, in design optimization, sensitivity coefficients due to uncertainty in nuclear cross-section data, material and geometric perturbation [6-9] can also be determined with variational methods. Good computational efficiency has been achieved for large-scale reactor design computations and with diverse applications in engineering [10]. For the optimal arrangement of fuel in a core, the Pontryagin Maximum Principle is used [3], to estimate the optimal control, i.e., best placement of high and low enriched fuel in the core. This constitutes an ODE-constrained optimization problem with the diffusion equation as the constraint. The drawback with variational methods has been their difficulty to be applied for large problems, for which Monte Carlo methods [11-13] and heuristic methods such as genetic algorithms have been demonstrated to be more attractive [14]. However, variational methods have been extended [7-9, 15] to thermal reactor physics calculations, with the computationally accelerated 3-D heterogeneous variational node method, amenable to parallelization. In the Monte Carlo method, sensitivity coefficients can be estimated by obtaining derivatives sampled in a single run thus, avoiding the need for performing an adjoint run in addition to a forward run, as is done in the deterministic approach. However, derivative sampling has been found to be accurate for small...
perturbations and hence, the choice of a reference condition has bearings on the computational efficiency of an optimization simulation. This work explores the computational advantage of using a variational result as an educated guess for starting a Monte Carlo derivative sampling simulation. Initial variational results are obtained from two-group neutron diffusion equations for illustrative examples of a two-zone reactor core, and a non-multiplying medium. In the formulation of this optimal control problem with the material density as the control variable, the Lagrangian is used since the effect of material distribution on the response of interest has a direct and an indirect component. The former due to the material density change and the latter due to the change in the field function i.e., the neutron flux, due to the change in density. As an example, the two-group theory is matched with the detailed MCNP5 [16] simulation results to strengthen its validity and enable its use to generalize on the applicability of its results.

This work presents a useful insight into the different approaches and is applicable to design optimization in nuclear systems.

**VARIATIONAL FORMULATION**

In design optimization, one of the goals is to maximize some reaction rate, or performance index, with a constraint such as the neutron diffusion (or transport) equation

\[
\dot{M} \phi = 0 \quad (1a)
\]

In a two-group formulation [17]

\[
\dot{M} = \begin{bmatrix}
\dot{L}_1 & \Sigma_{f,2} \\
\rho \Sigma_{s,1-2} & \dot{L}_2
\end{bmatrix}
\]

Here we have assumed that fissile neutrons are produced in the thermal group (group 2) and appear in the fast group (group 1). The atomic density of the materials, for a non-uniform distribution, can be written as \(N(x) = f(x)N_\text{av}\), subject to \(\int_a^b f(x)dx = 1\) in some domain \(\Gamma \in (a, b)\) with appropriate boundary conditions. In eq. (1a), the flux vector is \(\phi = [\phi_1, \phi_2]^T\) and the operator is \(\dot{L}_k = \nabla D \phi_1 \nabla \phi_2 - \Sigma_{s,1-2} \phi_2\) \((k = 1, 2)\).

The variational formulations considered here have a continuous control \(u\), and a discrete control \(u\) having an admissible set of values corresponding to the minimum and maximum values \(u_{\text{min}}\) and \(u_{\text{max}}\), respectively.

In the continuous formulation, the Lagrangian is written as

\[
\mathcal{L} = R_k + <\phi^* \mathbb{T}, \dot{M} \phi>_L \quad (2)
\]

with an objective to obtain the optimal distribution \(u^*\) by seeking first-order variations for a stationarity condition.

In the discrete formulation, where the control is given a value, the equations become easier to solve. Then eq. 1(a) is written in state-space form for variables \(y_i\) expressed as

\[
y_i = f_i(y, u, x), i = 0, 1, 2, 3, 4
\]

with the performance index included.

The Hamiltonian is then written as

\[
H = \sum_{i=0}^4 \lambda_i f_i(y, u, x) \quad (4)
\]

which yields the stationarity conditions

\[
\dot{y}_i = f_i(y, u, x) = \frac{\partial H}{\partial \lambda_i}
\]

and the adjoint equations

\[
\dot{\lambda}_i = -\frac{\partial H}{\partial y_i}
\]

With solutions obtained for \(y_i\) and \(\lambda_i\), using the transversality boundary conditions, the Hamiltonian can be found in the form

\[
H = g(u, x) + h(x)
\]

and thus the shape of \(g(u, x)\), also referred to as the switching function, determines which of the admissible values of the control \(u\) are to be applied to maximize \(H\). Then, according to Pontryagin’s Maximum Principle

\[
H(y^*, u^*, x) \geq H(y, u, x) \quad (7)
\]

where \(u_{\text{min}} \leq u \leq u_{\text{max}}\).

We now consider two illustrative examples where the previous formulations are used to obtain optimal distributions.

**EXAMPLE 1: OPTIMAL FUEL ENRICHMENT**

In a nuclear reactor core, fuel of varying enrichment is used and placed in such a way that uniform burnup is achieved and minimum fuel is required for criticality. The optimization problem is thus formulated as follows: Given some maximum fuel enrichment \(u_{\text{max}}\), what is the best placement of fuel such that the reactor is critical with minimum fuel mass? This is formulated as follows: minimize \(R = < u >\) where \(u = \sum_2 = \gamma u' + \delta, \gamma = \sigma_a^{235} N^{235}, u' = N^5 / N^U \) (enrichment), \(\delta = N^\text{others} \sigma_{a, \text{others}}\) with the constraint of fixed \(N^U\) – total number of uranium atoms in the domain \(r \in (0, R)\) subject to the constraint of eq. 1(a) with appropriate boundary conditions [3]. For a bare cylindrical reactor, the coupled second-order ODE representing the governing equation \(\dot{M} \phi = 0\) are written in state space form with the variables \(y_1 = \phi_1, y_2 = r \frac{d \phi_1}{dr}, y_3 = \phi_2, y_4 = r \frac{d \phi_2}{dr}\). The first-order equations are then
\[
\dot{y}_1 = y_2, \quad \dot{y}_2 = -\tau_1 y_2 + \tau_1 a u r y_3, \quad \dot{y}_3 = y_4, \quad \text{and} \quad \dot{y}_4 = -\tau_2 y_4 + \tau_2 b u r y_3 \quad \text{with} \quad y_0 = 2\pi a r \quad \text{added as a state equation. Here,} \quad \tau_1 = D_1 / \sum_1, \quad \tau_2 = p \sum_2 / D_2, \quad \alpha = k_s / pD_1, \quad \beta = l / D_2.
\]

These equations are solved using the transversality boundary conditions
\[
\lambda_1(R)\delta y_1(R) - \lambda_1(0)\delta y_1(0) = 0 \quad (8)
\]

for which the flux boundary conditions
\[
\phi_1|_{r=\delta} = \phi_1|_{r=0}, \quad \phi_1|_{r=\rho} = \phi_2|_{r=0} = 0 \quad \text{yield boundary conditions for the adjoint fluxes:}
\]
\[
\lambda_1|_{r=\delta} = \lambda_2|_{r=0} = 0 \quad \text{and} \quad \lambda_2|_{r=\rho} = \lambda_4|_{r=0} = 0.
\]

The Hamiltonian is now written in the form of eq. (6) with
\[
g(u, r) = u(2\pi a r 0 - \alpha r_2 y_3 + \beta r_4 y_3) \quad (9a)
\]
and
\[
h(r) = \frac{1}{\tau_1} \lambda_1 y_2 + \frac{1}{\tau_1} r_2 \lambda_2 y_1 + \frac{1}{\tau_2} \lambda_3 y_4 - \frac{1}{\tau_2} r_4 \lambda_4 y_1 \quad (9b)
\]
and thus the shape of \(g(u, r)\) also referred to as the \textit{switching function}, determines which of the admissible values of the control \(u\) are to be applied according to Pontryagin's Maximum Principle where \(u_{\text{min}} \leq u \leq u_{\text{max}}\).

The discrete form simplifies the continuous form by permitting the control \(u\) to be a constant in a particular sub-domain of the problem. Thus where \(g(u, x)\) is minimum (either sign), \(u_{\text{max}}\) is applied and vice versa. The number of zeros of the switching function will determine the number of controls applied. At the boundaries, \(g(u, 0) = 0\) and \(g(u, R) = 0\) with zeros in between. It can be inferred [3] that for the two-zone case, \(H\) is maximized with \(u = u_{\text{max}}\) in the first zone \(0 < r \leq R_1\) and \(u = u_{\text{max}}\) in the second zone \(R_1 < r \leq R\) where the zone boundary is at \(r = R_1\). While contrary to engineering practice of lower enrichment in the inner zone, this example is presented merely to demonstrate an optimal result. Similarly, for three zones, the maximization requirement is the control strategy \(u_{\text{min}}, u_{\text{max}}, u_{\text{min}}\) for the first, second and third zones, respectively. We thus need to find the critical pairs for each permissible value of \(u \leq u_{\text{max}}\). This is achieved from the criticality condition found by solving for the two-group fluxes using Cramer's rule \((\operatorname{det}(P) = 0)\) for homogenous

\[
\begin{bmatrix}
\lambda_1 S_{13} I_0(\lambda_1) & -\lambda_2 S_{23} I_1(\lambda_2) & -\lambda_2 S_{24} K_1(\lambda_2) \\
\lambda_1 S_{13} I_0(\lambda_1) & -\lambda_2 S_{23} I_1(\lambda_2) & -\lambda_2 S_{24} K_1(\lambda_2) \\
\end{bmatrix}
\]

Where \(J_0, \ Y_0\) are Bessel functions of order zero of first and second kind, and \(J_0, K_0\) are modified Bessel functions of the first and second kind, respectively. Here, \(S_{\text{ij}}\) are the coupling coefficients for zone \(i\) and index \(j\) with

\[
S_{11} = \tau_2 (\mu^2 + \beta u) = S_{21} = S_{22} \\
S_{13} = -\tau_2 (\lambda^2 - \beta u) = S_{23} = S_{24} \\
\mu^2 = \frac{1}{2\tau_1 L^2} \left( - (\tau_1 + \lambda^2) + \sqrt{(\tau_1 + \lambda^2)^2 + 4(k_u - 1)\tau_1 L^2} \right) \\
\lambda^2 = \frac{1}{2\tau_1 L^2} \left( (\tau_1 + L^2) + \sqrt{(\tau_1 + L^2)^2 + 4(k_u - 1)\tau_1 L^2} \right)
\]

For the three-zone case, Lee [3] has obtained a \(10 \times 10\) determinant.

We consider a bare homogeneous nuclear reactor core (radius 122.6 cm, height 365.8 cm) with the following two-group data [17]

\[
D_1 = 1.13 \text{ cm}, \quad \Sigma_s = 0.0419 \text{ cm}^{-1} \\
D_2 = 0.16 \text{ cm}, \quad \sigma_a^{215} = 678 b \\
N^U = N^{235} + N^{238} = 6994 10^{21} \text{ atoms per cm}^3
\]

Clearly, no optimal arrangement can be determined from the one-zone case as the bare reactor is found to be critical for a uniform enrichment of 1.1 % (critical mass 518.7 kg \(U^{235}\)). For a two-zone equal-volume \((R = 86.6913 \text{ cm}, 122.6 \text{ cm})\) configuration, the critical enrichment pairs found from the determinant are given in tab. 1. As the fuel enrichment in the first zone increases from natural uranium (\(u_{\text{max}} = 0.71\%\) to 1.2 %, the enrichment decreases in the second zone. With these combinations, the average \(u\) (a measure of the minimum critical mass) is given in the third row while MCNP results are given in the fourth row.
Table 1. Two-zone enrichment pairs for criticality

<table>
<thead>
<tr>
<th>$u_{\text{max}}/u_2$</th>
<th>0.71</th>
<th>0.9</th>
<th>1.1</th>
<th>1.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{\text{max}}/u_1$</td>
<td>1.54</td>
<td>1.27</td>
<td>1.1</td>
<td>1.01</td>
</tr>
<tr>
<td>$u_{\text{max}}$</td>
<td>1.13</td>
<td>1.09</td>
<td>1.1</td>
<td>1.13</td>
</tr>
<tr>
<td>MCNP</td>
<td>0.96760 (0.00397)</td>
<td>0.96538 (0.00190)</td>
<td>1.00422 (0.00192)</td>
<td>1.03035 (0.00169)</td>
</tr>
</tbody>
</table>

Table 2. Critical pairs, relative critical mass, MCNP runs

<table>
<thead>
<tr>
<th>Zone</th>
<th>DTPMP</th>
<th>MCNP (500 1 10 500)*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$u_{\text{min}}$ [%]</td>
<td>RCM</td>
</tr>
<tr>
<td>1.14</td>
<td>1.040</td>
<td>0.9797</td>
</tr>
<tr>
<td>1.13</td>
<td>1.042</td>
<td>0.9869</td>
</tr>
<tr>
<td>1.12</td>
<td>1.053</td>
<td>0.9869</td>
</tr>
<tr>
<td>1.11</td>
<td>1.067</td>
<td>0.9914</td>
</tr>
<tr>
<td>1.10</td>
<td>1.087</td>
<td>1.0</td>
</tr>
</tbody>
</table>

* (500 1 10 500) – means 500 neutrons simulated with an eigenvalue guess of 1 for 500 cycles with 10 skip cycles.

There are no solutions for $u_{\text{max}} \geq 1.2$ because at an enrichment of 1.2 %, the critical radius is less than the radius of the first zone. The MCNP runs for 1000 neutrons per cycle and 100 cycles give a preliminary estimate of $k_{\text{eff}} = 1.00195$ (0.00190) for 1.2 % enrichment with a bare cylindrical reactor of radius 68.05 cm and height 365.80 cm. The feasible solution for an optimal is thus the range 1.1-1.2 % enrichment in the first zone.

Two-group criticality pairs found from eq. 10(b) are given in tab. 2 along with the relative critical masses and corresponding MCNP simulations for 500 neutrons per cycle for 500 cycles and 10 skip cycles.

Assuming that the maximum available enrichment is 1.14 %, the minimum relative critical mass found is 0.9797 (508.18 kg U$^{235}$).

The masses in both zones are related as follows

$$M_2^{235} = u_1 V_1 M_1^{235}$$

so that the relative critical mass (RCM) is defined as

$$\text{RCM} = \frac{M_1^{235} + M_2^{235}}{M_0^{235}}$$

where $M_0^{235}$ = mass of U$^{235}$ in zone 1, $u_i$ = enrichment in zone 1, $V_i$ = volume of zone 1, $M_1^{235}$ = mass of U$^{235}$ in zones 1 and 2 for 1.1 % uniform distribution (518.7 kg).

The problem with increased enrichment in the central core is the enhanced fuel peaking which is not desirable and hence, less enriched fuel is placed in the central core. The present result is correct within the limitations of the two-zone model considered. Here, the total mass increases as lower enriched fuel is placed in the central core, as shown in fig. 1.

Figure 2 shows the thermal fluxes obtained from MCNP for three cases viz 1.1 % uniform enrichment, and small perturbations: 1.07 %-1.3 % and 1.13 %-1.04 % enrichments showing clearly the flattening of the thermal flux with a lower inner zone enrichment.

The criticality pairs can be computed from MCNP simulations by carrying out runs for each case which is clearly computationally expensive. This can be avoided by using the perturbation capability of MCNP5 [11] for sampling first- and second-order derivatives in a two-term Taylor series which can be used to estimate $k_{\text{eff}}$ for perturbations in the enrichment in terms of a reference $k_{\text{eff}}(u_0)$

$$k_{\text{eff}}(u) = k_{\text{eff}}(u_0) + \frac{\partial k_{\text{eff}}}{\partial u} \Big|_{u_0} \delta u + \frac{1}{2!} \frac{\partial^2 k_{\text{eff}}}{\partial u^2} \Big|_{u_0} (\delta u)^2 + \ldots$$

This formulation is suitable for optimization analyses which require the ability to estimate the effect of small changes such as in material density or geometry.

Thus, the first derivatives is computed as

$$c_1 = \frac{\partial k_{\text{eff}}}{\partial u} \Big|_{u_0} = \frac{k_{\text{eff}}(u) - k_{\text{eff}}(u_0)}{\delta u} = \left( \frac{\delta k}{\delta u} \right)$$

and the second derivative as
Further, the good reference condition provided by preliminary variation results show that estimates from both first- and second-derivatives, labelled FS for zones 1 and 2 in fig. 3(a), are only slightly better than the first derivative estimates, labelled F.

The previous analysis can readily be extended to three zones for which Pontryagin’s Maximum Principle gives a \( u_{min} \), \( u_{max} \), \( u_{min} \) which agrees better with Goertzel’s condition for flat thermal flux, as being the condition for minimum critical mass according to diffusion theory. The results for the two-zone case are to illustrate the variational formulation which gives a maximum value for the Hamiltonian (eq. 7) for a \( u_{max} \), \( u_{min} \) configuration.

EXAMPLE 2: NON-UNIFORM DENSITY IN A FIXED SOURCE SYSTEM

Similar to the previous example, in a fixed-source nuclear system, non-uniform material density may be considered for both elements and mixtures (with constituent elements) with the objective of increasing some reaction rate or decreasing the size of the system. For such an optimization problem, it would be desirable to obtain the optimal material distribution. Such a problem could use the continuous form of the variational formulation. With \( R_k = \sum_n \phi_n > 0 \) and \( \sum_k = N(x)\sigma_k = u(x)\sigma_k \), the Lagrangian is

\[
\mathcal{L} = \langle u \sigma_l^T \phi + \phi \phi^T \rangle_M \phi
\]

with an objective to obtain the optimal distribution \( u^* \) by seeking first-order variations for a stationarity condition.

With variations in \( u, \phi, \phi^* \) and \( \dot{M} \) and requiring the variations in the trial functions to be zero in the domain (excluding the boundary) we get for slab geometry

\[
\dot{L}_1^i \phi_i^+ + u(x)\sigma_{r,i} \phi_i^+ = 0 \tag{12a}
\]

\[
\dot{L}_2^i \phi_{i+} + u(x)\sigma_x \phi_{i+} = 0 \tag{12b}
\]

\[
\sum_{j=1}^{N} \frac{1}{\sigma_{r,j}} \left( \int \frac{1}{N} \frac{d\phi_{j}^+}{dx} \right) \phi_i^+ + \left( \frac{d}{dx} \frac{1}{N^2} \frac{d\phi_{j}^+}{dx} \right) \phi_i^+ = 0 \tag{12c}
\]

The previous formula are solved to give the fluxes

\[
\phi_1(x) = A_1 e^{\gamma_1 \int u(x)dx} + A_2 e^{-\gamma_1 \int u(x)dx} \tag{13a}
\]

\[
\phi_2(x) = A_3 e^{\gamma_2 \int u(x)dx} + A_4 e^{-\gamma_2 \int u(x)dx} + \mathcal{M} \phi_1(x) \tag{13b}
\]
\[ \phi_i^+(x) = A_2 e^{\gamma_2^+ u(x)} dx + A_4 e^{\gamma_2^- u(x)} dx + \left( \phi_i^+(x) - \frac{\sigma_{u,i}}{\sigma_{r,i}} \right) + \frac{\sigma_{u,i}}{\sigma_{r,i}} \] (13c)

\[ \phi_i^- (x) = A_2 e^{\gamma_2^+ u(x)} dx + A_4 e^{\gamma_2^- u(x)} dx + \frac{\sigma_{u,i}}{\sigma_{r,i}} \] (13d)

where \( \gamma_i = \sqrt{3\sigma_{r,i} \sigma_{u,i}}, \quad \sigma = \frac{\sigma_{r,i}}{\sigma_{r,2}} \left[ 1 - \left( \frac{\omega_{r,i}}{\omega_{r,2}} \right)^2 \right]^{-1} \)

Equations 13(a)-13(d) can be inserted in eq. 12(c) to get the optimal distribution \( u^*(x) \).

In the test problem, a slab of water thickness 20 cm is considered with a unit source of energy corresponding to group 1. In this case the control variable is the number density \( N(x) \) subject to the constraint of fixed total material. The performance index is the \((n,\gamma)\) reaction rate \( R_{H(n,\gamma)} \) of zone-averaged neutron flux in water and it is investigated whether the change in material distribution results in an optimum PI. The boundary conditions are thus

\[ J_1 (x = 0) = -D_1 \frac{d\phi_1}{dx} \bigg|_0 = \frac{S}{2} \]

and

\[ \phi_1 (x = L) = \phi_2 (x = 0) = \phi_2 (x = L) = 0 \]

Validation is carried out by computing two-group fluxes for material density uniform, linearly increasing and linearly decreasing as shown in fig. 4.

For the previous three cases, results are shown in fig. 5 where the gradual rise, then fall, in the group-2 fluxes is seen.

Figure 5 shows the effect of the density on group fluxes. It is seen that both 'move towards the right' for

the case of linearly increasing material distribution. These are compared with diffusion theory results shown in fig. 6.

All three cases are shown in fig. 7 (diffusion theory fluxes), where the left and right shift of the decreasing and increasing densities is seen.

Corresponding to the three cases, the PI is shown in fig. 8 with the trend mentioned earlier, i.e., a gradual shift towards the right for linearly increasing density.

To estimate the currents and subsequent doses, MCNP5 simulations were carried out for a slab (20 cm \( \times \) 10 cm \( \times \) 10 cm) containing water, with a 1 MeV neutron source incident on the left face (along the +x-axis) of thickness of 20 cm. The front and back surfaces were considered to be reflecting surfaces. The quantities tallied with MCNP5 were i- currents (neutron F1:n and photon F11:p tallies) emitted from the right face of

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**Figure 4.** Material density distribution considered for uniform distribution, linearly decreasing and linearly increasing distribution

**Figure 5.** Neutron fluxes with MCNP5 in group 1 (\( E > 5 \) eV) and group 2 (\( E \leq 5 \) eV), and \((n,\gamma)\) reaction rate in water; \( \langle \phi_i \rangle \) is the zone-averaged neutron flux in energy group \( i \); subscripts \( o, d, u \) refer to uniform-density, linearly decreasing, linearly increasing density

**Figure 6.** Neutron fluxes with two-group diffusion theory compared with MCNP in group 1 (\( E > 5 \) eV) and group 2 (\( E \leq 5 \) eV)
the slab, ii- dose equivalents in Sieverts (neutron and photon using dose equivalent factors), and iii- the reaction rates $R_i(n, \gamma)$ in cells of thickness 2 cm each in two energy bins ($E_1 \leq 5$ eV and $5$ eV $\leq E_2 \leq 1$ MeV). The results for $NPS = 10^5$ with a PHYS: P cutoff at 100 keV (PHYS: P 100 1 1) which took 5.14 minutes on an Intel(R) Core i7-2620M CPU at 2.70 GHz 32 bit operating system, are given in tab. 3.

Since 1 Sv = 100 rem, the neutron dose is $-6.3 \times 10^{-9}$ rem h$^{-1}$ for 1 source neutron per second; thus a neutron source of $10^5$ s$^{-1}$ would result in a (transmitted) neutron dose of 63 mrem h$^{-1}$ compared with the ICRP recommended maximum of 20 mSv per year (2 rem per year or 0.22 mrem h$^{-1}$). Without a water shield, a person at a distance 22 cm away would be receiving about 1000 times i.e., $\sim 63$ rem h$^{-1}$.

The reaction rate $R_{(h, \gamma)}$ from the F14:N tally is 2.94552 $10^{-4}$ (0.0034) cm$^{-3}$; the total volume is 2200 cm$^3$ and thus $R_{(h, \gamma)} = 0.6480$ reactions per source neutron per second. Thus, for a source $10^9$ neutrons per second, assuming one $\gamma$ produced per radiative capture, the $\gamma$ production in the water slab would be 0.6480 $10^9$ gammas per second. Less than 1% of these would be produced from group 1 (high energy) captures; thus the reaction rate is almost entirely from group 2 (lower energy) as expected from nuclear cross-section data.

It is seen from the MCNP5 results, in tab. 4, that a linearly decreasing density distribution (subject to constraint of fixed available material) gives an increase of $\sim 4%$ in the gamma production and $\sim 1%$ increase in the transmitted photon current and no significant increase ($\sim 1%$) in the transmitted neutron current, compared with the uniform case. Out of all three, the decreasing density case leads to (a slight) enhanced photon production with enhanced transmittance.

Exact solutions were obtained for the two-group neutron fluxes, eq. 13(a) and eq. 13(b), for three cases viz: $u(x) = \text{const.}$, $u(x) \sim 1/x$, and $u(x) \sim x$.

The group constants used for water are listed in tab. 5. In the present work, the data was obtained using a correction factor in which $\sigma_{u,2,2}$ were modified to 0.5004 b and 90 b from 0.58869 b and 99.185 b, respectively, taken from Lamarche and Barrata [17].

The molecular density of water in 3.3461 $10^{22}$ molecules per cm$^3$ and, for case i (uniform density), the mean free paths are 2.9688 cm and 0.1107 cm, respectively, with $D_1 = 1.13$ cm, $L_1 = 5.1961$ cm, $D_2 = 0.1107$ cm, $L_2 = 2.5711$ cm, $\tau = 27$ cm$^2$ and diffusion area $-6.61$ cm$^2$. Further, to match DT and Monte Carlo results for the PI for case i (uniform distribution), $\sigma_{\gamma f} = 87.475$ b.

Since MCNP5 does not have options to generate group cross-sections [18], these two-group cross-sections can be obtained by using group fluxes $\phi_i$ and associated reaction rates $<\sigma, \phi_i>$ where the inner product $<...>$ implies integration over the energy group of interest), and setting the group cross-section, for group $i$, as $\sigma_i^{(g)} = <\sigma, \phi_i>/\phi_i$.

The existing methodology for obtaining multi-group cross-sections is based on reading ENDF pointwise cross-section data, by processing codes such as NJOY (LANL) and MC2-3 (ANL) to produce binned cross-sections for use in multi-group deterministic codes. This is achieved by the group flux-weighting mentioned above and accounting for resonances and self-shielding.

The PI’s for cases i-iii are

### Table 3. Transmitted neutron and photon dose

<table>
<thead>
<tr>
<th></th>
<th>F1:N</th>
<th>F2:N (Dose)</th>
<th>F1:P</th>
<th>F2:P (Dose)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutrons</td>
<td>Sv</td>
<td></td>
<td>Photons</td>
<td>Sv</td>
</tr>
<tr>
<td>1.67067 $\times 10^{-7}$ (0.0177)</td>
<td>4.10858 $\times 10^{-13}$ (0.00562)</td>
<td>1.6866 $\times 10^{-7}$ (0.0085)</td>
<td>1.6222 $\times 10^{-10}$ (0.0123)</td>
<td></td>
</tr>
</tbody>
</table>
Table 4. Tallies for varying material distribution

<table>
<thead>
<tr>
<th>Material</th>
<th>N(x)</th>
<th>F1:N</th>
<th>Dose [Sv]</th>
<th>(n, g) avg [cm⁻³ s⁻¹]</th>
<th>F1:P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Decreasing</td>
<td>1.72933 x 10⁻⁷ (0.0174)</td>
<td>4.89229 x 10⁻¹³ (0.0580)</td>
<td>3.03990 x 10⁻¹⁴ (0.0033)</td>
<td>1.74480 x 10⁻¹⁰ (0.0084)</td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>1.71458 x 10⁻⁷ (0.0175)</td>
<td>4.25899 x 10⁻¹³ (0.0563)</td>
<td>3.00075 x 10⁻¹⁴ (0.0033)</td>
<td>1.71930 x 10⁻¹⁰ (0.0084)</td>
<td></td>
</tr>
<tr>
<td>Increasing</td>
<td>1.65803 x 10⁻⁷ (0.0180)</td>
<td>4.84695 x 10⁻¹³ (0.0605)</td>
<td>2.98457 x 10⁻¹⁴ (0.0033)</td>
<td>1.69710 x 10⁻¹⁰ (0.0085)</td>
<td></td>
</tr>
</tbody>
</table>

Table 5. Two-group cross-sections

<table>
<thead>
<tr>
<th>Data/Group</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>σ₁ [b]</td>
<td>1.2508</td>
<td>0.5004</td>
</tr>
<tr>
<td>σ₂ [b]</td>
<td>8.8158</td>
<td>90</td>
</tr>
</tbody>
</table>

\[
PI_1 = N_0 \left[ A_1 x \left( \frac{L_2}{L_1} - A_{11} x \right) - \omega_0 A_{11} x \right] + \frac{\omega_a}{\omega_0} A_{11} x \left( \frac{L_2}{L_1} - \omega_0 A_{21} x \right) \]

\[
PI_2 = A \left[ \frac{\beta_1}{\beta_2} A_{32} x \frac{\beta_1}{\beta_2} + A_{42} x \left( \frac{\beta_1}{\beta_2} + \omega A_{12} x \right) - \omega A_{22} x \left( \frac{\beta_1}{\beta_2} \right) \right] \]

\[
PI_3 = A \left[ A_1 I_1 \left( \frac{\beta_1}{2} \right) + A_2 I_1 \left( \frac{\beta_1}{2} \right) + \omega A_{12} I_1 \left( \frac{\beta_1}{2} \right) \right] \]

where

\[
\omega_0 = \frac{\sigma_{r,1}}{\sigma_{r,2}} \left( 1 - \frac{L_2}{L_1} \right) \]

\[
\omega_a = \frac{\sigma_{r,1}}{\sigma_{r,2}} \left( 1 - \left( \frac{\beta_1}{\beta_2} \right)^2 \right) \]

The design of multilayered concrete with aggregates (mainly gravel) is bound together by cement (mainly lime or calcium oxide, silica aluminium oxide) and water into a hard stone-like material with the required strength for structures such as buildings, bridges, roads etc. The relative composition of its constituents can be varied to provide the required mechanical e. g., the strength of concrete varies inversely with the mass ratio of water to cement. While Type 04 appears to be representative [19] with \( \rho = 2.35 \text{ gcm}^{-3} \), high-density concrete is made by mixing additives like scrap metal and magnetite. Piotrowski et al. [20] have carried out simulations for 25 cm thick wall of concrete of varying compressive strength to find that the effective dose behind the shield decreases up to 44 % as the compressive strength increases from 30 MPa (4351 psi) to 60 MPa (8702 psi) with water-cement (w-c) ratio 0.72 to 0.31. In other studies [21] the effect of boron in concrete has been studied to find that the optimal mixture of thermal neutron shielding concrete has a water-cement ratio of 0.38, cement content of 400 kgm⁻³, a volume fraction Colemanite aggregate of 50 % and silica fume-cement ratio of 0.15.

<table>
<thead>
<tr>
<th>N(x)</th>
<th>PI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lin. Dec.</td>
<td>0.63651</td>
</tr>
<tr>
<td>Uniform</td>
<td>0.64801</td>
</tr>
<tr>
<td>Lin. Inc.</td>
<td>0.63651</td>
</tr>
</tbody>
</table>
Similarly, the effect of another strong absorber, gadolinium, has been studied [22] to find that in concrete Gd content up to 10 at.% concrete composite (10 cm × 5 cm thick) shielding efficiency of around 86 %. For multi-layered iron-water shields [23] the optimum arrangement reported is the thick iron-water-thin iron configuration, rather than a homogeneous mixture of iron and water layers. Optimization for shields has also been used with Genetic Algorithms [24] for the search for an optimal radiation shield configuration subject to a given set of constraints. A number of innovations such as nanomaterials in concrete have also been investigated [25].

Multi-layered detector shields

Another problem of practical application, is for detection systems for materials' identification by thermal neutron activation [26]. For such systems, 252Cf has been used as a neutron source with emissions of 2.4 × 1012 s⁻¹ g⁻¹. In detectors, especially portable detection systems, size and weight are crucial and hence an optimal design is of paramount importance. Light weight hydrogenous materials such as polyethylene, paraffin and water are thus good candidates for neutron shielding compared with heavy materials such as steel and lead.

The variational formulations presented are readily applicable for obtaining optimal radiation shield designs for the above cases.

CONCLUSIONS

In the first illustrative example for variational application in Monte Carlo, a two-zone optimality analysis yielded the condition for minimum critical mass with maximum fuel enrichment in the central zone and minimum enrichment in the outer zone. This information was used in a detailed Monte Carlo simulation which, in a single run, estimated first- and second-derivatives for prediction of k-eff for enrichment perturbations in both zones. These predicted estimates were subsequently used to estimate the minimum condition which was predicted to within 1 % of the re-run estimate, clearly demonstrating the benefit of using a variational estimate for computational enhancement of an elaborate MCNP simulation. Such an approach can, in principle, be used for larger problems.

In the second illustrative example, a continuous variational formulation was attempted to estimate the benefit of a non-uniform density distribution for a single material. It was found that an exact solution was not achievable and recourse would again be required for a discrete approach, as in the first example. However, it was possible to estimate the perturbation resulting from non-uniformity. The application of this approach to the design optimization of radiation shields was discussed.

Both examples illustrate the advantage in using preliminary variational results from two-group diffusion equations, as an initial guess in a MC perturbation strategy to yield reliable estimates.

NOMENCLATURE

\( b \) – barn (10⁻²⁸ m²)
\( D_i \) – diffusion coefficient for group i
\( H \) – Hamiltonian
\( i \) – energy group index
\( k_c \) – infinite multiplication factor
\( u \) – control variable
\( u' \) – enrichment
\( J \) – current, \( J_i = -D_i N \phi_i \)
\( L \) – slab width
\( L_i \) – diffusion length for group i
\( \hat{L}_i \) – differential operator for energy group i
\( L^* \) – adjoint operator
\( M \) – molecular (atomic) weight
\( \tilde{M} \) – two-group operator
\( N \) – atomic density
\( N_T \) – total number of atoms (=NV)
\( N_o \) – \( \rho N_v / M \)
\( N_{av} \) – Avogadro's number (6.023 × 10²³ atoms/g-atom)
\( \rho \) – resonance escape probability
\( R_e \) – reaction rate for reaction type k
\( V \) – volume

Greek symbols

\( \lambda \) – Lagrange multiplier
\( \mathcal{L} \) – Lagrangian
\( \rho \) – gram density
\( \sigma_k \) – microscopic cross-section for reaction k
\( \tau \) – neutron age
\( \phi_i \) – neutron flux for energy group i
\( \phi_i^* \) – adjoint flux (Lagrange multiplier)
\( \Sigma_1 \) – macroscopic scattering cross-section (group 1)
\( \Sigma_2 \) – macroscopic absorption cross-section (group 2)
\( \Sigma_k \) – macroscopic cross-section for reaction k
\( \Sigma_{sc \rightarrow 1} \) – macroscopic scattering cross-section
\( \text{grp } 1 \rightarrow 2 \)

Abbreviations

DT – diffusion theory
DTPMP – diffusion theory Pontryagin maximum principle
ENDF – Evaluated Nuclear Data File
F1:N/P – current tally for neutrons/photon
F2:N/P – surface tally for neutrons
ICRP – International Commission on Radiological Protection
NPS – number of particles simulated
PI – performance index
PMP – Pontryagin maximum principle
rem – Roentgen equivalent man (traditional unit)

AUTHORS’ CONTRIBUTIONS

The mathematical modeling for variational and perturbation in the reactor core was carried out by Z. Koreshi and H. Khan, while the variational modeling for fixed-source was carried out by all three authors. Research was reviewed by all three authors.

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ВАРИЈАЦИЈИОНИ МЕТОДИ И УБРЗАЊЕ МОНТЕ КАРЛО ПРОРАЧУНА ПЕРТУРБАЦИЈА РАДИ ОПТИМАЛНОГ ДИЗАЈНА НУКЛЕАРНИХ СИСТЕМА

Потрага за оптималном расподелом материјала у нукларном систему ради максимизације функције одзива од интереса, тема је од значаја у области нукларног инжењерства. Неки од примера су оптимална расподела горива у језгру нукларног реактора како би се остварило унформио сагоревање коришћењем минимума критичне масе, или примена композитних материјала са оптималном смешом градивних елемената у детекторским системима или у заштити од зрачења. Варијационе методе корисне су за овајке прорачуне, али су коришћене само за појединачне анализе често ограничене на идеализоване модели, док су за детаљније пројектовање биле потребне компјутерски захтевне Монте Карло симулације неподобне у итеративним оптимизационим шемама. Ова инхерентна мана Монте Карло метода промењена је са развојом пертурбационих алгоритама, али је њихова ефикасност и даље зависна од референције конфигурације за коју се метода погоди-и-пробај често користи. У првом илустративном примеру у овом раду, испитује се убрзање прорачуна за голо цилиндрично језгро реактора, добијено примцем варијационог резултата како би се побољшала ефикасност прорачуна Монте Карло симулација оптимизације дизајна. У другом примеру, приказан је утицај неуинформне густине материјала у фиксно позиционираном извору, који је примењен за прорачун оптималног модератора и заштиту од зрачења. Иако су употребе овог приступа бројне, циљ овог рада је да прикаже прелиминарне варијационе резултате као улазне податке за разраду стохастичке оптимизације Монте Карло симулација за велике и реалне система.

Кључне речи: варијационе методе, оптимална расподела, Монте Карло пертурбација, нукларни система, минимална критична маса