A MONTE CARLO NORMALIZED DIFFUSION METHOD FOR CRITICALITY ANALYSIS OF SPENT FUEL STORAGE LATTICES

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ABSTRACT

A coupled Monte Carlo–diffusion theory model for the criticality analysis of spent fuel lattice configurations was previously presented by Rahnema et al. [1]. The model is based on two-group nodal diffusion in the context of the generalized equivalence theory (GET) [2]. The nodal parameters are determined from continuous energy Monte Carlo computations. The node-averaged diffusion coefficient is estimated by using an iterative technique.
In the present paper, a new method, based on a genetic algorithm, is proposed for calculating the node-averaged diffusion coefficient to be used in the nodal diffusion model. The unknown diffusion coefficients in each group and region of the lattice cell are to be estimated such that the multiplication constant of the fine-mesh diffusion calculation at the lattice cell level matches the result obtained from the Monte Carlo simulation of that cell. Two approaches are considered for modeling the spent fuel assembly when generating the nodal parameters: one in which the assembly is homogenized, and one in which the geometry of the assembly is modeled in full detail. The method is tested on a 2-D benchmark configuration typical of a spent fuel storage rack at Savannah River Site [3]. The accuracy of the nodal model is shown to be close to that of the continuous-energy Monte Carlo technique.

1. INTRODUCTION

Both deterministic and Monte Carlo transport codes have been used in nuclear criticality safety to determine the safety limits of spent fuel storage configurations. However, the Monte Carlo codes have been preferred because of their capability of modeling complex geometries and their continuous energy treatment of the neutron transport. A new computational tool was proposed by Rahnema et al. [1] as an alternative to the current methods used for estimating the subcriticality of spent fuel storage lattices. It is based on two-group nodal diffusion theory in the context of GET, and the nodal parameters (homogenized cross section and discontinuity factors) are determined by using Monte Carlo techniques. The node-averaged diffusion coefficient in the thermal group is approximated as $1/(3\Sigma_{tg})$, where Σ_{tg} is the node-averaged total cross section for group g; the node-averaged diffusion coefficient in the fast group is estimated by using an iterative procedure [1]. In this paper, a new method for estimating the node-averaged diffusion coefficient to be used in the nodal diffusion model is presented. When generating the nodal parameters for each unique

lattice cell type, two approaches are considered for modeling the lattice cell geometry: one in which the fuel assembly is homogenized (the current practice in the industry), and one in which its geometry is fully modeled.

2. METHOD

2.1. THE NODAL DIFFUSION MODEL

The nodal diffusion model presented in reference 1 is discussed in this section for completeness. The computation of the homogenized cross section and discontinuity factors is analyzed in more detail.

In the two-group 2-D nodal diffusion model, a water basin used to store spent fuel assemblies is modeled as a regular lattice (see Figure 1). Each lattice cell, consisting of the fuel assembly immersed in water and the water separating the fuel assemblies from each other, is treated as a homogenized node (see Figure 2). The node coupling is treated in the context of GET.

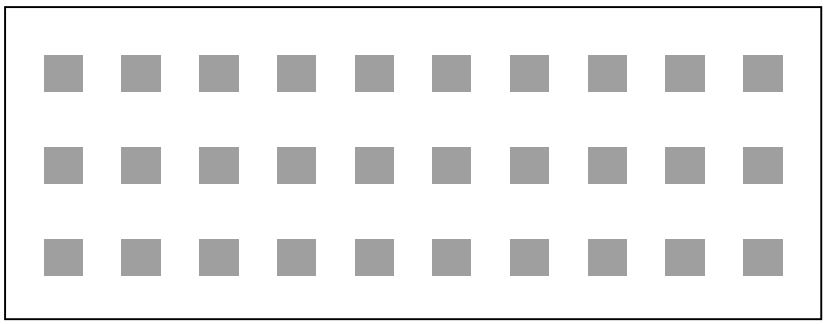


Figure 1. Storage Rack Configuration

GET [2] permits the conservation of both the reaction rates and the surface currents in the homogenization process by relaxing the continuity of flux condition at the node interface when solving the nodal equations. The flux at the interface is allowed to be discontinuous, and the relationship between fluxes on each side of the interface is expressed by using coupling parameters called discontinuity factors. The discontinuity factor f^k on side k of a node is defined as:

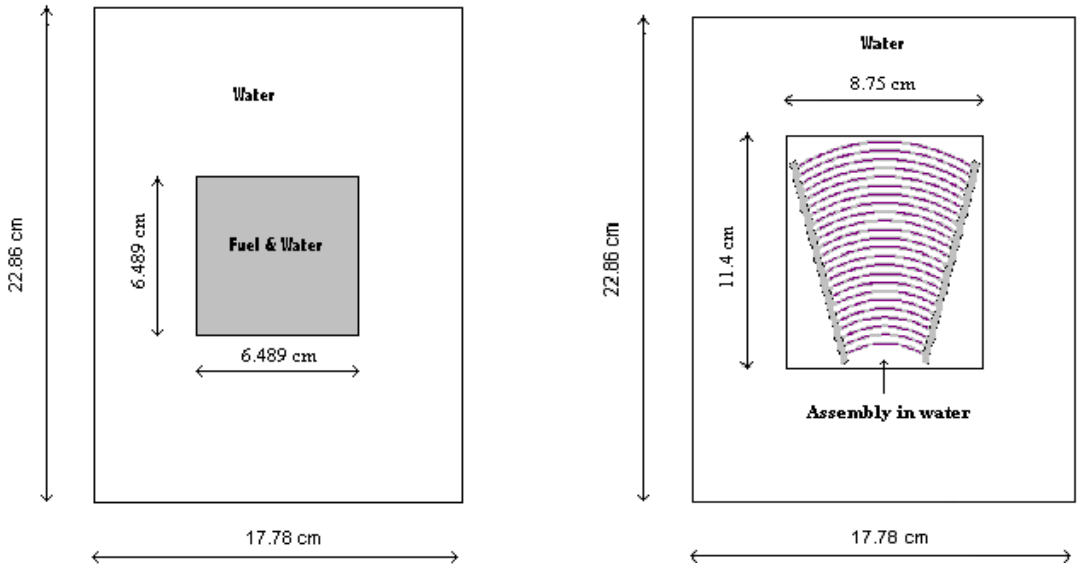
$$f^k = \frac{\overline{\psi}^k}{\overline{\varphi}^k} \tag{1}$$

where $\overline{\psi}^k$ is the surface-averaged heterogeneous flux (that is continuous at the interface) and $\overline{\varphi}^k$ is the surface-averaged homogeneous flux on that side. Given that the boundary condition for each node is not a priori known, the homogenized cross sections and discontinuity factors are approximated from single node calculations with zero current

boundary condition, also called infinite medium calculations. The infinite medium discontinuity factors are determined as [4]:

$$f^k = \frac{\overline{\varphi}^k}{\overline{\varphi}} \tag{2}$$

where $\overline{\varphi}$ is the node-averaged homogeneous flux.



a) conservative geometry modeling (MIT assembly type)

b) detailed geometry (MURR assembly type)

Figure 1. Typical Lattice Cell Configuration

In the nodal diffusion model [1], the two-group homogenized cross sections and discontinuity factors are precomputed for each assembly type (lattice cell type) from a MCNP [5] simulation of the lattice cell with a reflective boundary condition. The homogenized cross section in group g, $\overline{\Sigma}_g$, is calculated as:

$$\overline{\Sigma}_g = \frac{\int_g dE \int_{node} d^3 r \Sigma(\vec{r}, E)\varphi(\vec{r}, E)}{\int_g dE \int_{node} d^3 r \varphi(\vec{r}, E)} \tag{3}$$

where $\vec{r}$ and E are the space and energy variables, respectively, and φ is the scalar flux. The numerator in the above equation is obtained from a reaction rate tally, and the denominator from a flux tally in MCNP. The discontinuity factor is calculated as the ratio of the surface-averaged to the cell-averaged flux tallies (see Eq. 2).

2.2. CALCULATION OF THE NODE-AVERAGED DIFFUSION COEFFICIENT

In the present paper, the node-averaged diffusion coefficient, a key parameter in accounting for the node-to-node leakage, is calculated by using a genetic algorithm (GA). For a two-group, two-region description of the lattice cell (see Figure 2) with reflective boundary conditions, the following problem is considered: given the value of the multiplication constant (k_{MCNP}) from a continuous energy MCNP simulation of the lattice cell, determine the diffusion coefficient for each group and region such that the multiplication constant of the fine-mesh diffusion calculation at the cell level is the same (the neutron balance is conserved). This would be equivalent to considering the eigenvalue (k_{diff}) of the system (lattice cell) as a function of four unknowns (the diffusion coefficients) to be determined such that a particular solution ($k_{diff} = k_{MCNP}$) is obtained. This can be looked at as an optimization problem, with (k_{diff} - k_{MCNP}) as the objective function (i.e. to be minimized) and the diffusion coefficients as decision variables. Given the nonlinearity of the problem, a genetic algorithm (GA) is used to solve for the diffusion coefficients.

In the nuclear engineering field, stochastic optimization methods (such as simulated annealing or genetic algorithms) have been successfully applied in nuclear fuel management studies [6,7,8], as well as for neutron spectra unfolding [9]. A genetic algorithm is an optimization method based on the theory of biological evolution by natural selection. It deals with a population of potential solutions for a function optimization problem. The population of solutions is allowed to evolve under specific rules, by repeated applications of specific operators (selection, recombination, mutation), so that it tends to a state that optimizes an objective function [10,11,12].

The function to be optimized here is represented by:

$$f(p_1, p_2, p_3, p_4) = \left| k_{diff}(p_1, p_2, p_3, p_4) - k_{MCNP} \right| \tag{4}$$

where each parameter p_i corresponds to the diffusion coefficient in each group and region of the lattice cell, k_{MCNP} is the multiplication constant obtained from the MCNP simulation of the lattice cell with a reflective boundary condition, and k_{diff} is the multiplication constant obtained from infinite medium diffusion calculations for that lattice cell. The cross sections for each group and region used in the fine-mesh diffusion calculations for evaluating the function f are determined as in section 2.1.

The population of potential solutions for this optimization problem is represented by a finite number of strings, each composed of four numbers (the diffusion coefficients in each group and region):

$$c_i = \left[p_1^i, p_2^i, p_3^i, p_4^i \right] \qquad i = 1, size \tag{5}$$

The population is initialized by randomly selecting, for each component of each string c_i, a value in its domain of variation:

$$p_k^i = \alpha(hi_k - lo_k), \qquad k = 1,4 \qquad i = 1, isize \tag{6}$$

where α is a random number between 0 and 1, hi_k and lo_k representing the upper limit and the lower limit, respectively of the range for parameter p_k. For the current problem the exact range is not known. It is chosen such that:

$$5\left(\frac{1}{3\Sigma_t^k}\right) \le p_k \le 10^{-1}\left(\frac{1}{3\Sigma_t^k}\right) \tag{7}$$

where Σ_t^k is the total cross section in the same group and for the same region as that corresponding to p_k. Then the population is sorted by evaluating the function $f(c_i)$ (also called the "fitness" function) for each c_i and arranging the string in a list according to the value of the corresponding $f(c_i)$, from the smallest to the largest.

The population of solutions is allowed to evolve under specific rules, by repeated applications of specific operators. It is kept ranked by fitness at each step of the iterative process, such that the first string in the list at each moment of the evolution is the one that assures the best solution of the optimization problem at that moment. The selection (or pairing) is based on a simple approach: from top to bottom of the list of strings ranked after their fitness, two consecutive strings are chosen as a pair (e.g., first with second, third with fourth, and so on).

The recombination operator is applied to the pair of strings (called "parents") to combine them, such that to obtain two new strings or two possible solutions ("offspring") as a combination of the parent strings. A blending method (Radcliff's) [11] is used here for recombination, with the blending done for only one parameter in the string. Let c_m and c_d be the two strings in the pair subjected to recombination, with:

$$\begin{aligned} c_m &= \left[p_1^m, p_2^m, \ldots \quad p_k^m, \ldots \quad p_N^m\right] \\ c_d &= \left[p_1^d, p_2^d, ,\ldots \quad p_k^d, \ldots \quad p_N^d\right] \end{aligned} \tag{8}$$

where N is the length of the string (here N=4). First a crossover point to exchange information between c_m and c_d is chosen, by randomly selecting an integer on the interval [1, 4]. Let k be this integer. The offspring are obtained as:

$$\begin{aligned} c_{new}^1 &= \left[p_1^m, p_2^m, \ldots \quad p_{k-1}^m, p_k^{new,m}, p_{k+1}^m, \ldots \quad p_N^m\right] \\ c_{new}^2 &= \left[p_1^d, p_2^d, ,\ldots \quad p_{k-1}^d, p_k^{new,d}, p_{k+1}^d, \ldots \quad p_N^d\right] \end{aligned} \tag{9}$$

with

$$\begin{aligned} p_k^{new,m} &= \alpha p_k^m + (1-\alpha) p_k^d \\ p_k^{new,d} &= (1-\alpha) p_k^m + \alpha p_k^d \end{aligned} \tag{10}$$

where α is a random number on the interval [0, 1].

A random change in the solution is allowed through the mutation operator, so avoiding a premature convergence of the problem and therefore minimizing the chance that the search will end up in a local rather than in a global minimum. The operator is applied to the total population of parents and offspring with a size of 60. The number of parameters to suffer a mutation is found by multiplying the mutation rate by the number of strings and by the number of parameters in each string. The mutation rate used for the present problem is 2.5%, so there are six parameters that are changed (mutated). The string which it belongs to and the position in that string of the mutated parameter are selected randomly. The mutation consists of replacing the actual value of the parameter with another value, randomly selected from its domain of variation (between hi_k and lo_k).

After the mutation, the population of parents and offspring is reduced to the initial size ("culling") by removing the unfitted solutions, with a chance of survival of 2%. Starting from the bottom of the list of strings ranked after their fitness strings are removed, with a 2% probability for a string to be passed. When the size is reduced to half of the initial one, the process is stopped. If the top of the list is reached before removing half of the initial number of strings, the process is continued starting again from the bottom of the list back up to the top.

The new population is subjected to pairing, recombination, mutation and culling and the process continues until convergence is achieved. This is equivalent to requiring the value of the fitness function, evaluated for the first string in the list of strings ranked by their fitness, to be less than or equal to a smallness parameter:

$$f(c_1) = \left| k_{diff}(c_1) - k_{MCNP} \right| \le \varepsilon \tag{11}$$

Here 5×10^{-4} is used for the smallness parameter. For all unique lattice cell types analyzed, no more than ten iterations were required to achieve convergence. After the best solution (the values of the four diffusion coefficients) is determined, the two group diffusion coefficients for the node are calculated as:

$$D_g^{-1} = \frac{\sum_{i=1}^{2} D_{g,i}^{-1} \overline{\varphi}_i V_i}{\sum_{i=1}^{2} \overline{\varphi}_i V_i} \tag{12}$$

where D is the diffusion coefficient, $\overline{\varphi}$ the average flux, V the volume, and the indices i and g (i, g = 1,2) stand for region and group, respectively.

3. RESULTS

The benchmark configuration is a spent fuel storage rack [3] consisting of a 3x10 matrix of fuel assemblies in water. Two different arrangements of the assemblies in the storage rack are analyzed, and four types of fuel assemblies are considered. The fuel assembly is typical

of a research reactor, made up of thin metal plates of highly enriched uranium with aluminum cladding, held together by aluminum side plates. Two of the fuel assembly types, MIT and MURR, are typical of the Massachusetts Institute of Technology Reactor and University of Missouri Research Reactor, respectively [13]. The other two assemblies, TEST1 and TEST3, have a similar geometry, but the uranium content is purposely increased to create highly heterogeneous storage rack configurations. The material composition for each assembly type is shown Table I.

Table I. Material specification for the inner [a] region

Assembly Name	K_∞ [b] (σ_{rel})	U-235 (10^{24} at / cm^3)	U-238 (10^{24} at / cm^3)	Al (10^{24} at / cm^3)	H (10^{24} at / cm^3)	O (10^{24} at / cm^3)
MIT	0.60512 (0.00031)	5.5058e-04	3.7792e-05	1.9113e-02	4.4469e-02	2.2235e-02
MURR	0.72772 (0.00044)	4.7388e-04	3.2527e-05	2.5321e-02	3.7951e-02	1.8976e-02
TEST1	0.81004 (0.00049)	2.0000e-03	1.0284e-04	2.2116e-02	4.3278e-02	2.1639e-02
TEST3	0.95415 (0.00046)	1.0000e-02	1.0284e-04	2.2116e-02	4.3278e-02	2.1639e-02

[a] Conservative geometry modeling of the fuel assembly
[b] Infinite medium multiplication constant from continuous-energy MCNP

For each assembly type (considered homogenized), the nodal parameters are generated as discussed in the previous section. These parameters are used in performing the nodal diffusion calculations for the storage rack. The multiplication constant of the nodal calculation for each storage rack configuration is compared to the value obtained from a continuous-energy MCNP simulation of that configuration (see Table II). All MCNP calculations are performed by using continuous energy cross section libraries based on ENDF/B-V data files. It can be seen from Table II that the nodal diffusion calculation is in very good agreement with MCNP for all configurations: within 0.5% for the homogeneous rack configurations, and within 0.9% for the heterogeneous rack configurations. Note that some of the rack configurations are highly heterogeneous, such as the MIT (k_∞=0.6051) and TEST3 (k_∞=0.9541) lattice cell types arranged in a checkerboard pattern.

To assess the effect of the conservatism in modeling the assembly geometry (as a homogenized region) and the applicability of the proposed method in the case of a complex geometry lattice cell, the MURR assembly type (see Figure 1) is modeled in its full detail when generating the homogenized diffusion coefficients and cross sections. Two different compositions of the fuel are considered: fresh and depleted [14], to have two different types of the lattice cell. The multiplication constant of the nodal calculation for different arrangements of these two lattice cell types in the rack configuration are compared to the corresponding result obtained by simulating the configuration with the assembly's full detail (heterogeneity) with MCNP (see Table III). The agreement between the nodal diffusion results and those from MCNP is also very good in this case (within 0.6%).

Table II. K_{eff} for Spent Fuel* Rack 2-D Configurations

Rack Configuration	Assembly Type	K_{MCNP} (σ_{rel})	K_{nodal}	Δ^c (mk)	Δ^d (%)
Homogeneous [a]	MIT	0.58925 (0.00036)	0.58778	-1.5	-0.25
	MURR	0.70440 (0.00044)	0.70306	-1.3	-0.19
	TEST1	078785 (0.00053)	0.78416	-3.7	-0.47
	TEST3	0.93443 (0.00063)	0.93225	-2.2	-0.23
Heterogeneous [b]	MURR + MIT	0.65137 (0.00042)	0.65205	0.7	0.10
	TEST1 + MURR	0.75568 (0.00036)	0.74968	-6.0	-0.79
	TEST3 + TEST1	0.88032 (0.00043)	0.87649	-3.8	-0.44
	TEST1 + MIT	0.71259 (0.00035)	0.71053	-2.1	-0.29
	TEST3 + MURR	0.86448 (0.00060)	0.85889	-5.6	-0.65
	TEST3 + MIT	0.83864 (0.00058)	0.83369	-5.0	-0.59
	TEST1+ MIT + MURR	0.71804 (0.00033)	0.71455	-3.5	-0.49
	TEST3 + MURR + TEST1	0.85455 (0.00041)	0.84823	-6.3	-0.74
	TEST3 + MIT + TEST1	0.84215 (0.00041)	0.83513	-7.0	-0.83
	TEST3 + MIT + MURR	0.83260 (0.00042)	0.82525	-7.3	-0.88

* conservative modeling of assembly geometry when generating the nodal parameters

[a] identical rectangular nodes, same assembly type in every node

[b] identical rectangular nodes; checkerboard arrangement when two assembly types are present, (1,2,3) sequence when three assembly types (1, 2, and 3) are present

[c] calculated as $K_{nodal} - K_{MCNP}$; 1mk = 0.001

[d] calculated as $100*(K_{nodal} - K_{MCNP})/ K_{MCNP}$

Table II. K_{eff} for Spent Fuel** Rack 2-D Configurations

Rack Configuration	Assembly Type	K_{MCNP} (σ_{rel})	K_{nodal}	Δ^d (mk)	Δ^e (%)
Homogeneous [a]	$MURR_f$	0.69130 (0.00055)	0.69385	2.5	0.37
	$MURR_d$	0.64308 (0.00042)	0.64500	1.9	0.30
Heterogeneous [b]	$MURR_f$ +$MURR_d$ [c1]	0.66901 (0.00044)	0.67120	2.2	0.33
	$MURR_f$ +$MURR_d$ [c2]	0.66876 (0.00044)	0.67185	3.1	0.46
	$MURR_f$ +$MURR_d$ [c3]	0.67402 (0.00044)	0.67777	3.7	0.56

** detailed modeling of assembly geometry when generating the nodal parameters
[a] identical rectangular nodes, same assembly type in every node
[b] identical rectangular nodes, two assembly types
[c1] checkerboard arrangement of the fresh (f) and depleted (d) MURR assembly types
[c2] arrangement f d f d f d f d f d / f d f d f d f d f d / f d f d f d f d f d
[c3] arrangement f f f f f f f f f f / d d d d d d d d d d / f f f f f f f f f f
[d] calculated as K_{nodal} - K_{MCNP} ; 1mk = 0.001
[e] calculated as 100*(K_{nodal} - K_{MCNP})/ K_{MCNP}

3. CONCLUSIONS

A new method of estimating the node-averaged diffusion coefficient is developed in conjunction with a coupled Monte Carlo - diffusion theory model for regular lattice configurations [1]. The Monte Carlo based diffusion model is based on nodal diffusion theory within the context of GET, with the nodal cross sections and discontinuity factors determined from MCNP calculations, as discussed in section 2. The diffusion coefficients, which are unknown, cannot be calculated directly from an MCNP simulation of the lattice cell with a reflective boundary condition, as it is done for the homogenized cross sections and discontinuity factors. The latter ones are determined by using the corresponding tallies for reaction rates and fluxes in MCNP. There is no unique method for determining the diffusion coefficients.

The method presented here considers the determination of the unknown diffusion coefficients for each group and region of the lattice cell as an optimization problem. The function to be optimized is the infinite medium multiplication constant of the fine-mesh diffusion calculation (k_{diff}) at the lattice cell level. The unknown diffusion coefficients are to be determined such that $\left|k_{diff} - k_{MCNP}\right| \le 5x10^{-4}$, where k_{MCNP} is the multiplication constant from the MCNP simulation of the lattice cell with a reflective boundary condition. A genetic algorithm is used to solve this nonlinear optimization problem. The node-averaged diffusion coefficient is calculated by flux-weighting the inverse diffusion coefficients of all the regions of the lattice cell.

Two approaches are used when generating the nodal constants (including the diffusion coefficients) with MCNP for a given type of the spent fuel lattice cell: one in which the fuel assembly is modeled as a homogenized region, and one in which the fuel assembly is modeled in its full detail. Use of these nodal constants in the nodal diffusion method leads to very good results for the storage rack. The effective multiplication constant of the nodal calculations are within 1% of the corresponding values obtained from the MCNP simulation of the configurations in all of the analyzed cases.

The accuracy of the nodal method with the nodal parameters calculated as shown in this work is excellent from the point of view of nuclear criticality safety. The method can be useful as a tool for the optimization of a spent fuel storage configuration without resorting to direct Monte Carlo calculations that can be time consuming from the point of view of both modeling and computation.

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