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Optimization of Material Distributions in Fast Reactor Cores

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An iterative optimization method based on linearization and linear programming is developed. The method can be used for the determination of the material distributions in a fast reactor which maximize or minimize integral reactor parameters that are linear functions of the neutron flux and the material volume fractions.

The method has been applied to the problems of optimization of the fuel distribution in a reactor of fixed power output, constrained power density, and constrained material volume fractions so as to obtain (a) a maximum initial breeding gain, (b) a minimum critical mass, and (c) a minimum sodium void reactivity. Under this realistic set of constraints, numerical results show that the same fuel distribution yields maximum breeding gain, minimum critical mass, minimum sodium void reactivity, and uniform power density.

INTRODUCTION

The selection of the optimum value of a reactor parameter according to a criterion of optimality is a recurring problem in reactor design. Optimization techniques can provide answers to such a problem, since they seek the optimum solution in a systematic way.

A growing number of applications are being reported in the literature. Goldschmidt and Quenon[1] used the Maximum Principle of Pontryagin to find the fuel distribution which minimizes the critical mass of a slab geometry fast reactor described by one-group diffusion theory and subject to the constraints that (a) the total thermal power be constant, (b) the power density be less than or equal to an upper limit, and (c) the fuel enrichment be bounded. Tabak[2] used a simplified reactor model and showed that linear or quadratic programming can be applied to the problem of optimization of reactor fuel recycle. Sauar[3] used linear programming to determine the optimal fuel allocation in a light water reactor so as to minimize unit fuel cost. Gandini, Salvatores, and Sena[4] developed a method based on generalized perturbation theory and on linear programming to optimize reactor integral parameters, linear or bilinear in the real and adjoint neutron fluxes. Russian workers[5-7] have reported development and application of a method based on linear perturbation theory and on linear programming.

In general, optimization techniques have been used in reactor physics and engineering either for

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[1] P. GOLDSCHMIDT and J. QUENON, *Nucl. Sci. Eng.*, **39**, 311 (1970).

[2] D. TABAK, *IEEE Trans. Nucl. Sci.*, **NS-15**, 60 (1968).

[3] T. O. SAUAR, *Nucl. Sci. Eng.*, **46**, 274 (1971).

[4] A. GANDINI, M. SALVATORES, and G. SENA, *J. Nucl. Energy*, **23**, 469 (1969).

[5] V. V. KHROMOV, A. M. KUZ'MIN, and A. A. KASHUTIN, *Sov. At. Energy*, **27**, 917 (1969).

[6] A. A. KASHUTIN et al., "Optimization of Fast Reactors Taking the Thermal, Strength and Physical Characteristics into Account," JPRS-48331, **2**, 438, Translation of CEMA Symposium on the Atomic Power Stations with Fast Reactors, Obninsk (1969).

[7] A. M. KUZ'MIN et al., *Sov. At. Energy*, **31**, 787 (1971).

the solution of specific problems, or under constraints which are too few in number and inadequate in scope, or with a number of neutron groups at most equal to two. In this study, an optimization method is developed which can be applied to a broad category of optimization problems with realistic constraints and many neutron groups. It is an iterative method based on linearization of the equations describing the system, use of finite element techniques, and linear programming. The method can be used to maximize or minimize integral reactor quantities which are linear functions of the neutron flux and the material volume fractions. It has been applied to the problems of optimization of the fuel distribution of a fast breeder described by multigroup diffusion theory and having fixed power output, constrained power density, and constrained material volume fractions so as to (a) maximize the initial breeding gain, (b) minimize the critical mass, and (c) minimize the sodium void reactivity. It can be applied to many other problems related to reactor control, economics, and safety. More constraints can be easily introduced. In comparison with earlier efforts, the use of finite elements renders the present work computationally more compact and therefore facilitates applications to a greater variety of practical problems. Without any loss of generality, the development of the method will be discussed in connection with the breeding optimization problem.

MATHEMATICAL STATEMENT OF THE PROBLEM

A typical fast reactor consists of a core of plutonium-enriched fuel surrounded by a blanket of depleted uranium which, in turn, is surrounded by a reflector-shield region. In the context of multigroup diffusion theory,[8] the i'th neutron group flux $\phi_i(\mathbf{r})$, the power density $P(\mathbf{r})$, the total thermal power W delivered by the reactor, and an "economist's breeding gain" BG (net production of fissile material per unit power delivered) are given by the relations

$$\nabla \cdot D_i(\mathbf{r})\nabla\phi_i(\mathbf{r}) - \Sigma_{a,i}(\mathbf{r})\phi_i(\mathbf{r}) - \sum_{h=i+1}^{N} \Sigma_{(i\to h)}(\mathbf{r})\phi_i(\mathbf{r}) + \sum_{h=1}^{i-1} \Sigma_{(h\to i)}(\mathbf{r})\phi_h(\mathbf{r}) + \frac{\chi_i}{k}\sum_{h=1}^{N} \nu_h\Sigma_{f,h}(\mathbf{r})\phi_h(\mathbf{r}) = 0 \quad , \tag{1}$$

$$P(\mathbf{r}) = \sum_{i=1}^{N} \{u_f(\mathbf{r})\Sigma_{f,i}^{fs} + [N_0 - u_f(\mathbf{r}) - u_m(\mathbf{r})]\Sigma_{f,i}^{fr}\}\phi_i(\mathbf{r}) \quad , \tag{2}$$

$$W = \int_V \sum_{i=1}^{N} \{u_f(\mathbf{r})\Sigma_{f,i}^{fs} + [N_0 - u_f(\mathbf{r}) - u_m(\mathbf{r})]\Sigma_{f,i}^{fr}\}\phi_i(\mathbf{r})\,d\mathbf{r} \quad , \tag{3}$$

and

$$BG = \frac{\int_V \sum_{i=1}^{N} \{[N_0 - u_f(\mathbf{r}) - u_m(\mathbf{r})]\Sigma_{\gamma,i}^{fr} - \Sigma_{a,i}^{fs}u_f(\mathbf{r})\}\phi_i(\mathbf{r})\,d\mathbf{r}}{W} , \tag{4}$$

where

$\phi_i(\mathbf{r})$ = neutron flux in group i

$D_i(\mathbf{r})$ = diffusion coefficient for group i

$\Sigma_{a,i}(\mathbf{r})$ = macroscopic absorption cross section for group i

$\Sigma_{(i\to h)}(\mathbf{r})$ = macroscopic downscattering cross section for transfer from group i to group h by elastic and inelastic scattering

k = k_{eff}

χ_i = fraction of neutrons born into group i

$\Sigma_{f,h}(\mathbf{r})$ = macroscopic fission cross section for group h

N = number of neutron groups

$u_f(\mathbf{r})$ = volume fraction of the fissile material

$u_m(\mathbf{r})$ = volume fraction of the moderating material

$\Sigma_{f,i}^{fs}$ = macroscopic fission cross section of pure fissile material for group i

$\Sigma_{f,i}^{fr}$ = macroscopic fission cross section of pure fertile material for group i

N_0 = fissile volume fraction plus fertile volume fraction plus moderator volume fraction

$\Sigma_{\gamma,i}^{fr}$ = macroscopic capture cross section of pure fertile material for group i

$\Sigma_{a,i}^{fs}$ = macroscopic absorption cross section of pure fissile material for group i

V = reactor volume.

The breeding optimization problem consists of finding the optimum fissile and moderator distributions $u_f(\mathbf{r})$ and $u_m(\mathbf{r})$, respectively, which maximize the breeding gain BG (Eq. 4), while the following conditions are satisfied:

[8] J. R. LAMARSH, *Introduction to Nuclear Reactor Theory*, Addison-Wesley Publishing Co., Inc., Reading, Massachusetts (1966).

1. The reactor is critical.
2. The power density $P(\mathbf{r})$ is bounded.
3. The total thermal power W is constant.
4. The sum of fissile and moderator volume fractions is bounded, namely $u_f(\mathbf{r}) + u_m(\mathbf{r}) \leq N_0 = \text{const}$.

THE LINEARIZED FORM OF THE BREEDING OPTIMIZATION PROBLEM

From Eqs. (1) through (4) it is seen that the optimization problem of interest is nonlinear. Application of the Maximum Principle of Pontryagin leads to a two-point boundary value problem which is difficult to solve either analytically or numerically, and which involves subtle questions concerning satisfaction of the equality part of inequality constraints. Dynamic programming, in spite of its conceptual and programming simplicity, imposes exceptionally large fast-access computer memory requirements.

These difficulties can be avoided through use of linear programming, for which standard computer routines are readily available. In the subsequent discussion, we will assume that the reader is familiar with the concepts, theorems, and terminology of linear programming and optimization theory discussed in standard texts (e.g., Ref. 9).

In general, linear programming is a method for maximizing (minimizing) a linear objective function for a system with linear algebraic constraints.[9] Accordingly, the nonlinear problem of interest can be reduced to a form suitable for use of linear programming in two steps:

1. The relations describing the problem are linearized.
2. The linearized relations are transformed into linear algebraic relations.

Linearization of Eqs. (1) through (4) is achieved by means of Taylor series expansions around a reactor operating point corresponding to any fuel and moderator distributions, $u_f^0(\mathbf{r})$ and $u_m^0(\mathbf{r})$, respectively, which satisfy the problem constraints. Thus, the following relations are obtained:

Linearized Multigroup Diffusion Equations

$$\nabla \cdot D_i^0(\mathbf{r})\nabla\phi_i^*(\mathbf{r}) - \Sigma_{a,i}^0(\mathbf{r})\phi_i^*(\mathbf{r}) - \sum_{h=i+1}^{N} \Sigma_{(i\to h)}^0(\mathbf{r})\phi_i^*(\mathbf{r}) + \sum_{h=1}^{i-1} \Sigma_{(h\to i)}^0(\mathbf{r})\phi_h^*(\mathbf{r}) + \chi_i \sum_{h=1}^{N} \nu_h \Sigma_{f,h}^0(\mathbf{r})\phi_h^*(\mathbf{r})$$

$$+ [u_f(\mathbf{r}) - u_f^0(\mathbf{r})]\left(-(\Sigma_{a,i}^{fs} - \Sigma_{a,i}^{fr})\phi_i^0(\mathbf{r}) - \sum_{h=i+1}^{N} [\Sigma_{(i\to h)}^{fs} - \Sigma_{(i\to h)}^{fr}]\phi_i^0(\mathbf{r}) + \sum_{h=1}^{i-1} [\Sigma_{(h\to i)}^{fs} - \Sigma_{(h\to i)}^{fr}]\phi_h^0(\mathbf{r})\right.$$

$$\left. + \chi_i \sum_{h=1}^{N} (\nu_h^{fs}\Sigma_{f,h}^{fs} - \nu_h^{fr}\Sigma_{f,h}^{fr})\phi_h^0(\mathbf{r}) - \nabla \cdot \left\{\frac{\Sigma_{tr,i}^{fs} - \Sigma_{tr,i}^{fr}}{3[\Sigma_{tr,i}^0(\mathbf{r})]^2}\right\}\nabla\phi_i^0(\mathbf{r})\right) + [u_m(\mathbf{r}) - u_m^0(\mathbf{r})]$$

$$\times \left(-(\Sigma_{a,i}^{m} - \Sigma_{a,i}^{fr})\phi_i^0(\mathbf{r}) - \sum_{h=i+1}^{N} [\Sigma_{(i\to h)}^{m} - \Sigma_{(i\to h)}^{fr}]\phi_i^0(\mathbf{r}) + \sum_{h=1}^{i-1} [\Sigma_{(h\to i)}^{m} - \Sigma_{(h\to i)}^{fr}]\phi_h^0(\mathbf{r})\right.$$

$$\left. + \chi_i \sum_{h=1}^{N} (-\nu_h^{fr}\Sigma_{f,h}^{fr})\phi_h^0(\mathbf{r}) - \nabla \cdot \left\{\frac{\Sigma_{tr,i}^{m} - \Sigma_{tr,i}^{fr}}{3[\Sigma_{tr,i}^0(\mathbf{r})]^2}\right\}\nabla\phi_i^0(\mathbf{r})\right) = 0 \tag{5}$$

Linearized Power Density

$$P(\mathbf{r}) = u_f(\mathbf{r}) \sum_{i=1}^{N} (\Sigma_{f,i}^{fs} - \Sigma_{f,i}^{fr})\phi_i^0(\mathbf{r}) - u_m(\mathbf{r}) \sum_{i=1}^{N} \Sigma_{f,i}^{fr}\phi_i^0(\mathbf{r}) + \sum_{i=1}^{N} \Sigma_{f,i}^0\phi_i^*(\mathbf{r}) + \sum_{i=1}^{N} N_0 \Sigma_{f,i}^{fr}\phi_i^0(\mathbf{r}) \tag{6}$$

Linearized Total Thermal Power

$$W = \int_V u_f(\mathbf{r}) \sum_{i=1}^{N} (\Sigma_{f,i}^{fs} - \Sigma_{f,i}^{fr})\phi_i^0(\mathbf{r})d\mathbf{r} - \int_V u_m(\mathbf{r}) \sum_{i=1}^{N} \Sigma_{f,i}^{fr}\phi_i^0(\mathbf{r})d\mathbf{r} + \int_V \sum_{i=1}^{N} \Sigma_{f,i}^0(\mathbf{r})\phi_i^*(\mathbf{r})d\mathbf{r}$$

$$+ \int_V \sum_{i=1}^{N} N_0\Sigma_{f,i}^{fr}\phi_i^0(\mathbf{r})d\mathbf{r} \tag{7}$$

[9] G. HADLEY, *Linear Programming*, Addison-Wesley Publishing Co., Inc., Reading, Massachusetts (1962).

Linearized Breeding Gain

$$BG = \frac{1}{W}\left(-\int_V u_f(\mathbf{r}) \sum_{i=1}^{N} (\Sigma_{\gamma,i}^{fr} + \Sigma_{a,i}^{fs})\phi_i^0(\mathbf{r})d\mathbf{r} - \int_V u_m(\mathbf{r}) \sum_{i=1}^{N} \Sigma_{\gamma,i}^{fr}\phi_i^0(\mathbf{r})d\mathbf{r}\right.$$
$$\left. + \int_V \sum_{i=1}^{N} \{[N_0 - u_f^0(\mathbf{r}) - u_m^0(\mathbf{r})]\Sigma_{\gamma,i}^{fr} - u_f^0(\mathbf{r})\Sigma_{a,i}^{fs}\}\phi_i^*(\mathbf{r})d\mathbf{r} + \int_V N_0 \sum_{i=1}^{N} \Sigma_{\gamma,i}^{fr}\phi_i^0(\mathbf{r})d\mathbf{r}\right) \quad , \tag{8}$$

where

$\phi_i^*(\mathbf{r}) = \phi_i(\mathbf{r}) - \phi_i^0(\mathbf{r})$

$\Sigma_{tr,i}^{fs}$ = macroscopic transport cross section of pure fissile material for group i

$\Sigma_{tr,i}^{fr}$ = macroscopic transport cross section of pure fertile material for group i

$\Sigma_{tr,i}^{m}$ = macroscopic transport cross section of pure moderating material for group i

$\Sigma_{a,i}^{m}$ = macroscopic absorption cross section of pure moderating material for group i

$\Sigma_{(i\to h)}^{m}$ = macroscopic downscattering cross section of pure moderating material for transfer from group i to group h.

The superscript "0" is used to denote quantities evaluated at the operating point about which the relations describing the reactor are linearized.

For the reactor to remain critical, the distributions $u_f(\mathbf{r})$ and $u_m(\mathbf{r})$ must satisfy a criticality condition which is mathematically complicated. The mathematical complications may be reduced by use of perturbation theory to express the criticality condition in the form[10]

$$-\int_V [u_f(\mathbf{r}) - u_f^0(\mathbf{r})] \sum_{i=1}^{N} \frac{\Sigma_{tr,i}^{fs} - \Sigma_{tr,i}^{fr}}{3[\Sigma_{tr,i}^0(\mathbf{r})]^2} \nabla\phi_i^0(\mathbf{r})\nabla\psi_i^0(\mathbf{r})d\mathbf{r} + \int_V [u_f(\mathbf{r}) - u_f^0(\mathbf{r})] \sum_{i=1}^{N} (\Sigma_{a,i}^{fs} - \Sigma_{a,i}^{fr})\phi_i^0(\mathbf{r})\psi_i^0(\mathbf{r})d\mathbf{r}$$
$$+ \int_V [u_f(\mathbf{r}) - u_f^0(\mathbf{r})] \sum_{i=1}^{N} \sum_{h=i+1}^{N} [\Sigma_{(i\to h)}^{fs} - \Sigma_{(i\to h)}^{fr}]\phi_i^0(\mathbf{r})[\psi_i^0(\mathbf{r}) - \psi_h^0(\mathbf{r})]d\mathbf{r} - \frac{1}{k}\int_V [u_f(\mathbf{r}) - u_f^0(\mathbf{r})]$$
$$\times \sum_{i=1}^{N} \sum_{h=1}^{N} (\nu^{fs}\Sigma_{f,h}^{fs} - \nu^{fr}\Sigma_{f,h}^{fr})\chi_i\phi_h^0(\mathbf{r})\psi_i^0(\mathbf{r})d\mathbf{r} - \int_V [u_m(\mathbf{r}) - u_m^0(\mathbf{r})] \sum_{i=1}^{N} \frac{\Sigma_{tr,i}^{m} - \Sigma_{tr,i}^{fr}}{3[\Sigma_{tr,i}^0(\mathbf{r})]^2} \nabla\phi_i^0(\mathbf{r})\nabla\psi_i^0(\mathbf{r})d\mathbf{r}$$
$$+ \int_V [u_m(\mathbf{r}) - u_m^0(\mathbf{r})] \sum_{i=1}^{N} (\Sigma_{a,i}^{m} - \Sigma_{a,i}^{fr})\phi_i^0(\mathbf{r})\psi_i^0(\mathbf{r})d\mathbf{r} + \int_V [u_m(\mathbf{r}) - u_m^0(\mathbf{r})]$$
$$\times \sum_{i=1}^{N} \sum_{h=i+1}^{N} [\Sigma_{(i\to h)}^{m} - \Sigma_{(i\to h)}^{fr}]\phi_i^0(\mathbf{r})[\psi_i^0(\mathbf{r}) - \psi_h^0(\mathbf{r})]d\mathbf{r} - \frac{1}{k}\int_V [u_m(\mathbf{r}) - u_m^0(\mathbf{r})]$$
$$\times \sum_{i=1}^{N} \sum_{h=1}^{N} (-\nu^{fr}\Sigma_{f,h}^{fr})\chi_i\phi_h^0(\mathbf{r})\psi_i^0(\mathbf{r})\,d\mathbf{r} = 0 \quad , \tag{9}$$

where

ψ_i = adjoint flux for group i.

The linearized relations (6) through (9) can be transformed into linear algebraic relations by dividing the reactor into a number of regions, R, each with spatially uniform material concentrations, and by solving the linearized multigroup diffusion equations so that each $\phi_i^*(i = 1, 2, \ldots, N)$ is expressed as a function of the fuel and moderator concentrations, $u_{f,j}$ and $u_{m,j}$, respectively, in the region $j(j = 1, 2, \ldots, R)$. Thus, the functional to be maximized and the constraints of the problem become linear algebraic functions of $u_{f,j}$ and $u_{m,j}$, and therefore suitable for application of linear programming.

SOLUTION OF THE LINEARIZED MULTIGROUP DIFFUSION EQUATIONS

The linearized multigroup diffusion equations are of the form

$$L\,\phi^* = f(u_f^*, u_m^*) \quad , \tag{10}$$

where L is the multigroup diffusion matrix operator and

$$u_f^* = u_f - u_f^0, \quad u_m^* = u_m - u_m^0 \quad . \tag{11}$$

[10] P. E. ROHAN, "Comparisons of Transport and Diffusion Theory Calculations of Performance Characteristics for Large Fast Reactors," PhD Thesis, University of Illinois, Urbana (1970).

We want to express ϕ^* as a function of u_f^* and u_m^*. Application of the finite difference technique gives a set of algebraic equations of the form

$$M\phi^* = f(u_f^*, u_m^*) \quad , \tag{12}$$

which can be solved by inversion of the matrix M. On the other hand, even for five neutron groups and 100 mesh points, M is a large (500 × 500) matrix; its inversion requires excessive computer time and gives rise to prohibitive roundoff errors.

This difficulty can be avoided by use of the method of finite elements discussed by Kang and Hansen.[11] To this end, the reactor is divided into a number n of mesh points and the flux difference ϕ_i^* is approximated by

$$\phi_i^* \simeq \Phi_i^* = \sum_{k=1}^{n} a_{k,i} w_k + \sum_{k=1}^{n} \beta_{k,i} v_{k,i} \quad , \tag{13}$$

where w_k and $v_{k,i}$ are cubic piecewise polynomials.[11] The coefficients $a_{k,i}$ and $\beta_{k,i}$ are determined by requiring

$$\int_V (L_i \Phi_i^*) w_k \, dV = \int_V f_i(u_f^*, u_m^*) w_k \, dV \tag{14}$$

and

$$\int_V (L_i \Phi_i^*) v_{k,i} \, dV = \int_V f_i(u_f^*, u_m^*) v_{k,i} \, dV \quad . \tag{15}$$

The integrations on the right sides of Eqs. (14) and (15) cannot be carried out since the space dependence of u_f^* and u_m^* is unknown. On the other hand, if the reactor is divided into R regions with spatially uniform material concentrations in each region, then the right sides of Eqs. (14) and (15) can be integrated and a system of algebraic equations results. These equations are of the form

$$Aa = g(u_f^*, u_m^*, a_{11}) \quad , \tag{16}$$

where a_{11} is the coefficient of the polynomial w_1 in Eq. (13) for $i = 1$, and the components of the vectors u_f^*, u_m^* are given by

$$\begin{aligned} u_{f,j}^* &= u_{f,j} - u_{f,j}^0 \quad , \\ u_{m,j}^* &= u_{m,j} - u_{m,j}^0 \quad , \\ j &= 1, 2, \ldots, R \quad . \end{aligned} \tag{17}$$

The solution of the system of Eq. (16) is of the form

$$a = A^{-1} g \quad . \tag{18}$$

For n mesh intervals and N neutron groups, the order of the matrix A is equal to $2nN - 1$. The method of finite elements, compared to the finite difference technique, gives a very good approximation to ϕ_i^* with only a few mesh intervals n. This results in a smaller matrix A than the finite difference technique for the same accuracy in ϕ_i^*. For example, for $N = 5$ and $n = 10$, the order of A is $2 \times 10 \times 5 - 1 = 99$. For the same accuracy in ϕ_i^*, the finite difference technique gives a 500×500 matrix.

THE ITERATIVE SCHEME

The solution of the linearized multigroup diffusion equations results in all constraints and the objective function of the problem being linear algebraic relations of $u_{f,j}$ and $u_{m,j}$ ($j = 1, 2, \ldots, R$). This means that the original nonlinear optimization problem has been reduced to a linear programming optimization problem.

The linearized form of the breeding optimization problem is a good approximation to the original nonlinear problem only if $u_{f,j}$ and $u_{m,j}$ are sufficiently close to $u_{f,j}^0$ and $u_{m,j}^0$ about which the linearization was performed. Therefore, linear programming can be applied to obtain the optimum values of $u_{f,j}$ and $u_{m,j}$ which maximize the objective function and are subject to the additional constraints

$$\begin{aligned} u_{f,j}^0 - \epsilon_f \le u_{f,j} \le u_{f,j}^0 + \epsilon_f \, , \\ u_{m,j}^0 - \epsilon_m \le u_{m,j} \le u_{m,j}^0 + \epsilon_m \\ (j = 1, 2, \ldots, R) \quad . \end{aligned} \tag{19}$$

The quantities ϵ_f, ϵ_m are such that $u_{f,j}$ and $u_{m,j}$ remain close enough to $u_{f,j}^0$ and $u_{m,j}^0$, respectively.

In general, this procedure results in a suboptimum solution, since $u_{f,j}$ and $u_{m,j}$ are restricted by Eq. (19) to only small variations around $u_{f,j}^0$ and $u_{m,j}^0$. The optimum solution can be found by means of the following iterative scheme. If $u_{f,j}^{(1)}$ and $u_{m,j}^{(1)}$ is the solution given by the first application of linear programming, the problem is relinearized about $u_{f,j}^{(1)}$, $u_{m,j}^{(1)}$, constraints (19) are replaced by the relations

$$\begin{aligned} u_{f,j}^{(1)} - \epsilon_f \le u_{f,j} \le u_{f,j}^{(1)} + \epsilon_f \, , \\ u_{m,j}^{(1)} - \epsilon_m \le u_{m,j} \le u_{m,j}^{(1)} + \epsilon_m \\ (j = 1, 2, \ldots, R) \quad , \end{aligned} \tag{20}$$

and linear programming is again applied to obtain another solution $u_{f,j}^{(2)}$, $u_{m,j}^{(2)}$, etc.

The procedure of linearization about the previous solution of linear programming and reapplication of linear programming is repeated until no further improvement of the objective function is achieved. The last linear programming solution gives the optimum fissile and moderator distributions which result in the maximum value

[11] C. M. KANG and K. F. HANSEN, "Finite Element Methods for Space-Time Reactor Analysis," MIT-3903-5, MITNE-135, Massachusetts Institute of Technology (1971).

of the objective function. Note that there is no assurance that the determined optimum is a local (relative) or a global (absolute) one. Therefore, the iterative procedure should be repeated, starting with different initial fissile and moderator distributions, and the determined optima compared.

Note that the necessity of proceeding in small steps does not restrict the method to initial operating points close to the optimum solution. Any starting point consistent with all constraints is satisfactory. Obviously, fewer iterations are required for judiciously selected starting configurations. In addition, the use of a succession of small steps distinguishes the present method from that of Ref. 4, in which a single large step is taken.

REMARKS

In principle, the optimization method developed can be applied to any reactor geometry. However, for geometries involving more than one dimension the method becomes very complicated in terms of its numerical implementation.

From among the possible one-dimensional geometries, infinite cylindrical geometry has been selected in this study because (a) cylindrical geometry is, almost without exception, characteristic of practical reactors, and (b) the optimization of either the fuel distribution or the moderator distribution or both is likewise of practical importance primarily in the radial direction. Nevertheless, the method can be applied equally well to any one-dimensional geometry.

In addition, note that many two-dimensional calculations in cylindrical geometry are approximated by one-dimensional calculations by adding to the macroscopic absorption cross section a DB^2 term to account for axial leakage.[12] This approximation can, and has, been incorporated in the present optimization method.

APPLICATIONS

The optimization method has been applied to the core of a 1500 MW(th) fast breeder to obtain the fuel distribution that (a) maximizes the initial breeding gain, (b) minimizes the critical mass, and (c) minimizes the sodium void reactivity.

For these studies, two reactors of infinite cylindrical geometry and four core regions of equal volume are considered. The dimensions of Reactor No. 1 are given in Table I, and its composition is given in Table II. This composition is representative of LMFBR design studies presented over the last several years.[13,14]

TABLE I

Dimensions of Reactor No. 1

Region		Inner Radius (cm)	Outer Radius (cm)
Core	1	0.00	62.64
	2	62.64	90.48
	3	90.48	111.36
	4	111.36	128.76
Radial blanket	5	128.76	174.00[a]

[a] Extrapolated outer boundary.

The sum of the PuO_2 and UO_2 volume fractions is constrained to remain constant during optimization and equal to 0.35.

For computational convenience, the total thermal power has been normalized to 100 and the power density limit (550 W/cm^3) to a corresponding value 2.30267.

For the neutronic calculations, five neutron groups were employed. The ANISN multigroup transport theory code was used to obtain a five-group cross section set by collapsing a sixteen-group modified Hansen-Roach cross section set.[15]

The three problems of breeding optimization, critical mass optimization, and sodium void reactivity optimization are described by the same equations, except for the objective function.

TABLE II

Reactor Composition

Material	Core (vol %)	Blanket (vol %)	Atomic or Molecular Density for Pure Materials (10^{24} cm^{-3})
Na	50	50	0.025410
Fe	15	15	0.084870
PuO_2	35	--	0.025189
UO_2		35	0.024444

[12] W. B. LOEWENSTEIN and G. W. MAIN, "Fast Reactor Shape Factors and Shape-Dependent Variables," ANL-6403, Argonne National Laboratory (1961).

[13] *Proc. Conf. Safety, Fuels and Core Design in Large, Fast Power Reactors,* ANL-7120, Argonne National Laboratory (1965).

[14] *Proc. Intern. Conf. Sodium Technology and Large Fast Reactor Design,* ANL-7520, Argonne National Laboratory (1968).

[15] G. E. HANSEN and W. H. ROACH, "Six and Sixteen Group Cross Sections for Fast and Intermediate Critical Assemblies," LAMS-2543, Los Alamos Scientific Laboratory (1967).

Table III presents the results obtained in the successive iterations of the iterative optimization method applied to the breeding optimization problem. The computation begins with a four-region homogeneous core as given by the first row of Table III. The optimum distribution is given by the last row of the same table. The breeding gain listed in the last column of the table is calculated by the relation

$$BG = \frac{2\pi \int_0^{t_f} \sum_{i=1}^{N} [(N_0 - u_f)\Sigma_{\gamma,i}^{fr} - \Sigma_{a,i}^{fs} u_f]\phi_i r dr}{2\pi \int_0^{t_f} \sum_{i=1}^{N} \Sigma_{f,i}\phi_i r dr}, \quad (21)$$

where

t_f = reactor radius.

The peaks of the power density in each core region (which occur at the inner radius of each region) for the initial and optimum distributions are shown in Table IV. Since, as already mentioned, there is no assurance that the determined optimum is a local or a global one, the optimization procedure was repeated with a different initial distribution. The same optimum distribution was obtained.

The results in Table III show that for the five-region reactor with dimensions as given in Table I (Reactor No. 1) the optimum distribution is one for which there is no PuO_2 in the fourth region, and the peaks of the power density in regions 1 and 2 are equal to the upper power density limit. The breeding gain of the optimum distribution is 4.08% larger than the breeding gain of the initial homogeneous distribution.

The optimization started with a reactor of four core regions and a 45.24-cm blanket. The optimum distribution consists of three core regions and 62.64-cm blanket. (PuO_2 was removed from the fourth core region of the initial distribution.) This suggests that a distribution resulting in a further improved breeding gain may be obtained by redivision of the core into four regions and reapplication of the optimization procedure. Thus, the core of the optimum Reactor No. 1 is redivided into four regions of equal volume. Since a typical fast reactor blanket is ~45 cm thick,[13,14] the extra blanket is also removed. The dimensions of the new reactor, which will be called Reactor No. 2 in the remainder of this study, are shown in Table V.

The composition and the peak power densities of the optimum distribution of Reactor No. 2 are shown in Table VI. The breeding gain of the optimum distribution is equal to 0.5825. As shown in Table VI, the peak power densities in the first three core regions of the optimum con-

TABLE III

Fissile Composition and Breeding Gain as a Function of Linear Programming Iteration Number for Reactor No. 1

Iteration Number	Region				Breeding Gain[a]
	1	2	3	4	
	PuO_2 (vol%)				
1	3.41200	3.41200	3.41200	3.41200	0.576527
5	3.33607	3.95874	2.61200	2.61200	0.583506
10	3.29407	4.15375	2.48842	1.61200	0.589804
15	3.28765	4.11576	2.86731	0.61200	0.594337
20	3.27801	4.08658	3.07689	0.00000	0.600585
21	3.27801	4.08662	3.07676	0.00000	0.600585

[a]Net production of ^{239}Pu atoms per fission. Expression of results to six figures is to permit proper appreciation of various aspects of numerical methodology, rather than to imply a high degree of accuracy.

TABLE IV

Relative Peak Power Densities for Reactor No. 1

Region	1	2	3	4
Initial distribution	2.23971	1.68232	1.15895	0.72096
Optimum distribution	2.30265	2.30264	1.14762	0.07654

TABLE V

Dimensions of Reactor No. 2

Region		Inner Radius (cm)	Outer Radius (cm)
Core	1	0.00	55.68
	2	55.68	80.04
	3	80.04	97.44
	4	97.44	111.36
Radial blanket	5	111.36	156.60[a]

[a]Extrapolated outer boundary.

TABLE VI

Optimum Configuration of Reactor No. 2

Region	1	2	3	4
PuO_2 vol%	3.23751	3.72338	5.01528	0.50175
Relative peak power density	2.30267	2.30267	2.30267	0.29742

figuration are all equal to the upper power density limit.

The breeding gain of the optimum configuration of Reactor No. 2 is slightly smaller than the breeding gain of the optimum configuration of Reactor No. 1. This is due to the fact that Reactor No. 2 is smaller than Reactor No. 1 and consequently loses more neutrons by leakage. Reduction of the leakage can be achieved by surrounding the blanket by a reflector. The breeding gain of the initial homogeneous version of Reactor No. 1, the optimum configuration of Reactor No. 1, and the optimum configuration of Reactor No. 2, before and after the addition of a 45.24-cm BeO reflector at the outer periphery of the blanket, are shown in Table VII. The optimum Reactor No. 2 now has a higher total breeding gain than the homogeneous Reactor No. 1 and the optimum Reactor No. 1, although it has a core ~25% smaller than the homogeneous Reactor No. 1. In addition, it is important to note that the optimum Reactor No. 2 has a lower *internal* breeding gain than the initial homogeneous version of Reactor No. 1, but a higher *total* breeding gain because of the high breeding efficiency of the typical LMFBR blanket.

The same optimization procedure was applied to the problems of critical mass optimization and sodium void reactivity optimization. For the problem of minimum critical mass, the objective function is given by the relation

$$M_c = \frac{A \times M^{Pu}}{N_A} \int_0^{t_f} 2\pi r\, u_f(r)\, dr \quad , \qquad (22)$$

where

A = atom density of plutonium in PuO_2

M^{Pu} = atomic weight of plutonium

N_A = Avogadro's number.

For the problem of minimum sodium void reactivity, the fuel optimization process is viewed as follows. The critical reactor, or part of it, is voided; consequently, the reactor becomes subcritical or supercritical. Then the question is raised as to how the fuel should be redistributed in the voided reactor so that (a) the k_{eff} of the voided reactor is minimized, and (b) if the sodium is brought back into the reactor, the reactor becomes critical, delivers the same power as before voiding, and the power density is everywhere less than or equal to a given upper limit.

If the fissile fuel distribution of the voided reactor is changed from $u_f^0(r)$ to $u_f(r)$ and if $u_f(r)$ is sufficiently close to $u_f^0(r)$, then perturbation theory gives the following expression for the change in k_{eff} of the voided reactor:

$$\begin{aligned}\frac{1}{k_v} - \frac{1}{k_v^p} = \left(\frac{1}{I}\right)\Bigg(-\int_0^{t_f} u_f^* \sum_{i=1}^{N} \frac{(\Sigma_{tr,i}^{fs} - \Sigma_{tr,i}^{fr})}{3(\Sigma_{tr,i}^0)^2} \nabla\phi_i \nabla\psi_i\, r dr \\ + \int_0^{t_f} u_f^* \sum_{i=1}^{N} (\Sigma_{a,i}^{fs} - \Sigma_{a,i}^{fr}) \phi_i \psi_i\, r dr \\ + \int_0^{t_f} u_f^* \sum_{i=1}^{N} \sum_{h=i+1}^{N} \\ \times \{[\Sigma_{(i\to h)}^{fs} - \Sigma_{(i\to h)}^{fr}]\phi_i(\psi_i - \psi_h)\} r dr \\ - \frac{1}{k_v} \int_0^{t_f} u_f^* \sum_{i=1}^{N} \sum_{h=1}^{N} \\ \times (\nu^{fs}\Sigma_{f,h}^{fs} - \nu^{fr}\Sigma_{f,h}^{fr})\chi_i \phi_h \psi_i\, r dr\Bigg) \quad , \qquad (23)\end{aligned}$$

where

$$I = \int_0^{t_f} \sum_{i=1}^{N} \chi_i \psi_i \left(\sum_{h=1}^{N} \nu\Sigma_{f,h}\, \phi_h\right) r dr$$

k_v = k_{eff} of voided reactor

k_v^p = k_{eff} of voided reactor after the fissile fuel perturbation.

The minimization of the sodium void reactivity is equivalent to the minimization of the quantity $(1/k_v) - (1/k_v^p)$ given by Eq. (23).

For the specific set of constraints applied, numerical results show that the fuel distribution which leads to a maximum breeding gain leads also to a minimum critical mass and a minimum sodium void reactivity. Specifically, the optimum Reactor No. 2 has a critical mass 30.50% and a

TABLE VII

Effect of Blanket Reflector on Breeding Gain

Reactor	Breeding Gain of Unreflected Reactor			Breeding Gain after Addition of BeO Reflector[a]		
	Internal	External	Total	Internal	External	Total
Homogeneous No. 1	0.405686	0.170841	0.576527	0.405832	0.202875	0.608707
Optimum No. 1	0.345045	0.255540	0.600585	0.345059	0.270237	0.615296
Optimum No. 2	0.377648	0.204880	0.582528	0.378024	0.239341	0.616365

[a] 45.24-cm-thick BeO reflector.

sodium void reactivity 2.9 dollars less than the initial homogeneous reactor.

As has been mentioned, two-dimensional calculations can be approximated by one-dimensional calculations by adding to the macroscopic absorption cross section an appropriate DB_z^2 term to account for axial leakage. The compositions, breeding gains, and peak power densities of the initial and optimum configurations of two cylindrical fast breeders having the same radial dimension as Reactors No. 1 and No. 2 are listed in Tables VIII and IX.

Axial leakage has been accounted for by adding to the macroscopic absorption cross section a region- and group-dependent DB_z^2 term. A value of 0.0004382 cm^{-2} was used for B_z^2. The breeding gain shown in Tables VIII and IX includes the internal (core) breeding gain and the external breeding gain of the radial blanket (i.e., axial blanket breeding gain is not considered). Comparison of Tables IV through IX shows that the optimum configurations of Reactors No. 1 and No. 2 with and without axial leakage are similar.

The computer program written to carry out the computations was not intended for use as a production program and hence has not been groomed to minimize storage requirements or running time. Typical running times for the results presented are of the order of 30 min on an IBM 360. The running time is proportional to the number of iterations required to go from the starting configuration to the optimum configuration. The number of iterations depends on how close the initial configuration is to the optimum configuration and on the value of the parameter ϵ [Eqs. (19) and (20)]. Control of errors in the linearized Eqs. (5) through (8) and the perturbation theory, Eq. (9), imposes on the parameter ϵ values such that the $u_{f,j}$, $(j = 1, 2, \ldots, R)$ remain close enough to $u_{f,j}^{0}$ [Eqs. (19) and (20)]. For the results of Table III, the value of $\epsilon = 0.002$ was used. Reduction of the value of the parameter ϵ to $\epsilon = 0.001$ approximately doubled the number of iterations and consequently the computer time required to go from the starting configuration of Table III to the optimum configuration. Values of $\epsilon > 0.002$ would reduce the computation time. However, for $\epsilon > 0.002$, the perturbation theory, Eq. (9), after a few iterations leads to a considerable drift of k_{eff} from its value in the starting configuration. In turn, such errors in k_{eff} lead to considerable errors in breeding gain. An approximate relation between the error in k_{eff} and the error in breeding gain can be derived by using one-group theory:

$$\delta BG \simeq -\nu\, \delta k_{\text{eff}} \simeq -3\, \delta k_{\text{eff}} \quad . \tag{24}$$

The optimization method has also been applied to the problem of optimization of the distribution of a moderator in a fast reactor blanket so as to obtain a maximum initial breeding gain. Numerical results indicate, however, that the initial breeding gain is a very weak function of the moderator concentration in the blanket; therefore, numerical errors are sufficiently large compared to changes in the optimization variables to obviate blanket optimization by this approach.

To support these results, the change of the

TABLE VIII

Optimum Configuration of Reactor No. 1 with Axial Leakage

Region		1	2	3	4	Breeding Gain
PuO_2 vol%	initial	3.99000	3.99000	3.99000	3.99000	0.2750
	optimum	3.83424	4.74201	3.61363	0.0	0.2948
Relative peak power densities	initial	2.2532	1.6884	1.1587	0.7158	
	optimum	2.3026	2.3026	1.1528	0.0730	

TABLE IX

Optimum Configuration of Reactor No. 2 with Axial Leakage

Region		1	2	3	4	Breeding Gain
PuO_2 vol%	initial	3.83400	4.20000	4.80600	4.04000	0.2671
	optimum	3.78963	4.32869	5.80107	0.61625	0.2829
Relative peak power densities	initial	2.2074	2.0820	1.8404	1.0748	
	optimum	2.3026	2.3026	2.3026	0.2972	

breeding gain as a function of the moderator concentration, homogeneously distributed, was investigated. The dimensions of an infinite cylindrical geometry reactor considered for the computation are shown in Table X. The reactor composition for BeO- and Na-moderated blankets are shown in Tables XI and XII, respectively. For the neutronic calculations, five neutron groups were used, having the same structure and with the same cross sections as for the previous problems.

The results presented in Table XIII show that for even marginally significant changes in the breeding gain large changes in the moderator volume fraction in the blanket are required. In addition, the results show the following:

1. When sodium replaces ^{238}U in the blanket, the neutron moderation by sodium is not enough to offset the loss in breeding due to reduction of the ^{238}U concentration; consequently, the breeding gain decreases as the sodium concentration increases.
2. When BeO replaces ^{238}U in the blanket, for a BeO volume fraction somewhere between 5 and 10% the improvement in breeding due to moderation by BeO just offsets the loss in breeding due to reduction of the ^{238}U concentration; for any other BeO concentration, the neutron moderation is not enough to offset breeding losses due to reduction of the ^{238}U concentration.

The results just cited support the conclusion of the optimization studies to the effect that the initial breeding gain depends weakly on the moderator volume fraction in the blanket.

TABLE X

Dimensions of Reactor Used in Blanket Studies

Region		Inner Radius (cm)	Outer Radius (cm)
Core	1	0.00	62.64
	2	62.64	90.48
	3	90.48	111.36
Radial blanket	4	111.36	160.08
Reflector	5	160.08	206.48[a]

[a]Extrapolated outer boundary.

SUMMARY AND CONCLUSIONS

An iterative optimization method based on linearization and on linear programming is de-

TABLE XI

Reactor Composition for BeO-Moderated Blanket

Material	Core Regions 1 (vol %)	2 (vol %)	3 (vol %)	Blanket	Reflector	Atomic or Molecular Density for Pure Materials (10^{24} cm^{-3})
PuO_2	3.2775	4.0859	3.0763	--	--	0.025189
UO_2	31.7225	30.9141	31.9237	55	--	0.024444
BeO	--	--	--		--	0.071270
Na	50	50	50	30	--	0.025410
Fe	15	15	15	15	100	0.084870

TABLE XII

Reactor Composition for Na-Moderated Blanket

Material	Core Regions 1 (vol %)	2 (vol %)	3 (vol %)	Blanket	Reflector	Atomic or Molecular Density for Pure Materials (10^{24} cm^{-3})
PuO_2	3.2775	4.0859	3.0763	--	--	0.025189
UO_2	31.7225	30.9141	31.9237	85	--	0.024444
Na	50	50	50		--	0.025410
Fe	15	15	15	15	100	0.084870

TABLE XIII

Breeding Gain as a Function of Moderator Concentration in the Blanket

Case	Moderator (vol %)	^{238}U (vol %)	Breeding Gain		
			Internal	External	Total
Na Moderator					
1	10	75	0.340401	0.286165	0.626566
2	20	65	0.341137	0.282633	0.623770
3	30[a]	55	0.342077	0.277693	0.619770
4	40	45	0.343326	0.270523	0.613849
5	50	35	0.345091	0.259680	0.604771
BeO Moderator					
6	0	55	0.342077	0.277693	0.619770
7	5	50	0.344532	0.275832	0.620364
8	10	45	0.347181	0.272908	0.620089
9	20	35	0.353354	0.263742	0.617096
10	30	25	0.361465	0.248656	0.610121
11	5[b]	50	0.344557	0.275206	0.619763
12	5[c]	50	0.343183	0.271740	0.614923

[a]The volume fractions of Na and UO_2 of this row are representative of typical fast reactor blanket designs.

[b]$\sigma^{BeO}_{(n,2n)} = 0.0$.

[c]$\sigma^{BeO}_{downscattering} = 0.0$.

veloped. The method can be used for the determination of the material distributions in a fast reactor of fixed power output, constrained power density, and constrained material volume fractions that maximize or minimize integral reactor parameters which are linear functions of the neutron flux and the material volume fractions.

The method has been applied to the following problems:

1. Optimization of fuel distribution in the reactor core so as to obtain (a) maximum initial breeding gain, (b) minimum critical mass, and (c) minimum sodium void reactivity. Under the specific constraints imposed, numerical results show that the same fuel distribution yields maximum breeding gain, minimum critical mass, minimum sodium void reactivity and uniform power density.

2. Optimization of a moderator distribution in the blanket so as to maximize the initial breeding gain. Results indicate that the breeding gain is a weak function of the moderator distribution. These results are confirmed by studying the effects on the breeding gain of the insertion of a moderator, homogeneously distributed, in the blanket.

Solutions of the minimum critical mass problem have frequently appeared in the literature.[1,16-21] These solutions, however, either do not consider constraints which are sufficiently realistic for practical reactor designs, or they use at most two neutron groups for thermal reactors and one neutron group for fast reactors. In this study, an improved solution to the minimum critical mass problem has been given for fast reactors having fixed power output, limited power density, and limited fuel concentration, and described by multigroup diffusion theory.

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