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The In-Core Fuel Management by Variational Method

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Abstracts

The in-core fuel management problem was studied by use of the calculus of variations. Two functions of interest to a public power utility, the profit function and the cost function, were subjected to the constraints of criticality, the reactor burnup equations and an inequality constraint on the maximum allowable power density.

The variational solution of the initial profit rate demonstrated that there are two distinct regions of the reactor, a constant power region and a minimum inventory or flat thermal flux region. The transition point between these regions is dependent on the relative importance of the profit for generating power and the interest charges for the fuel.

The fuel cycle cost function was then used to optimize a three equal volume region reactor with a constant fuel enrichment. The inequality constraint on the maximum allowable power density requires that the inequality become an equality constraint at some points in the reactor. and at all times throughout the core cycle. The finite difference equations for reactor criticality and fuel burnup in conjunction with the equality constraint on power density were solved, and the method of gradients was used to locate an optimum enrichment.

The results of this calculation showed that standard non-linear optimization techniques can be used to optimize a reactor when the inequality constraints are properly applied.

요 약

변분법을 사용하여 원자로의 핵연료 관리문제를 연구하였다. 원자력 발전소에 영향을 미치는 두 함수 즉 이윤함수와 가격함수는 원자로의 연소도방정식과 최대허용출력 밀도에 대한 부등 제약조건이며, 이들은 임계성의 제약조건이 된다.

초기이윤의 변분해는 원자로에 뚜렷한 두 영역이 있음을 보여 주었다. 즉 일정 출력 영역과 최소 재고량 또는 평활 중성자속 영역이 그것이다. 이들 두 영역의 변이점은 전력에 대한 이윤과 연료에 대한 이자 지급에 상당히 중요하다.

그러므로 각 영역에서 동일 농축도의 핵연료를 가진 동일 부피의 세 영역으로 된 원자로를 최적화하기 위하여 핵연료 주기 가격 함수가 사용 되었다. 최대 허용 출력 밀도에 대한 부등 제약조건들을

이들 부등 제약 조건이 원자로심의 어느 특정 점이나 로심주기를 통하여 항상 동일 제약조건이 되어야 한다. 원자로의 임계성과 출력밀도에 대한 동일 제약조건에 관계된 핵연료의 연소도에 대한 계차방정식의 해를 구하였으며 최적 농축도의 위치를 구하기 위하여 구배법을 사용하였다.

이들 계산결과는 부등 제약 조건들을 적절히 적용하면 원자로를 최적화 하기 위하여 비선형 최적기술이 사용될 수 있음을 보여 주었다.

I. Introduction

It is the purpose of this study to present the fuel management concerned with the choosing of enrichments and the placement of fuel assemblies into a fixed reactor. The obvious ultimate goal of the fuel management is to maximize the profit earned by a utility producing power. There are three basic aspects to this objective of maximization of profit; (1) One can utilize the fuel more completely by operating it to high burnups. (2) Inventory charges must be paid by the utility. If the interest rates are low, this may not be too severe a limitation. (3) Profit is earned by selling power. Therefore to maximize the utility's profit, it is necessary to operate the reactor at the highest possible power level.

Early work[1]~[3] in the fuel management was primarily concerned with achieving higher burnups in fuel. It was recognized that this could be achieved by refueling the reactor preferably continuously but more realistically in steps. Since there are many choices available to the fuel manager for discharging and rearranging fuel.

The most common schemes which were studied are: (1) Out-in management scheme, (2) In-out management scheme, (3) Roundelay or scatter loading to yield a uniform exposure, and (4) Batch loading in which all the fuel is discharged at the end of a core cycle. From these schemes it was found that out-in cycling gives acceptable results for small cores and the roundelay or scatter loading approach looked promising for large cores.

It has been found that the cycling approach yields low discharge burnups for the first two zones of a three zone core and a recent attempt to improve the burnups in three zones leads to the concept of "fuel sharing"[4]. In this approach fuel discharged from the first reactor is used in the start-up of a second reactor which is due to begin operation approximately two years after the first reactor is brought on the line. One half the fuel assemblies from core one are used, along with fresh fuel in the second unit and the second core of unit one has the same loading as the first core of unit two. Fuel discharged from the first cycle of these reactors has a higher net burnup which lowers the fuel cycle cost for the system of reactors.

In the PWR, it was found that to achieve minimum fuel cycle cost it is necessary to obtain a good power distribution at the beginning of the core cycle. An attempt to obtain a power distribution which is identical to the power distribution in the previous cycle is given by Melice[5]. He defines a pointwise k-distribution which is an infinite "transversal" multiplication factor including a term for the axial buckling, and maintains this k-distribution for all succeeding cycles.

Fegan[6] considered of optimizing the fuel reloading for the equilibrium cycle but did not consider the problem of approach to the equilibrium cycle. The dynamic programming technique has also been applied to the optimization of fuel management schemes. Wall[7] applied dynamic programming to a one enrichment three region PWR. It is noted that in these schemes it is necessary to perform an enumeration calculation in order to find an optimum

peaking factor.

In this paper, the variational calculus is used to obtain an optimal fuel distribution in a batch reactor. The profit functional, which is the dollar profit from burning a fuel isotope less interest charges for that isotope, is subjected to the constraints of criticality and the burnup equations with an inequality constraint on the maximum allowable power density. It is shown that the maximum profit is obtained by operating the reactor to peak power density at some points in the core, not necessarily the same point, at all times during the core cycle. This inequality constraint is then applied to a three region batch reactor and a three region out-in cycled reactor. It is shown that the optimum enrichment in these reactors can be found by the standard optimization techniquee of the gradient method and the Newton-Raphson method.

II. Mathematical Formalism

To analyze a problem by use of the calculus of variationals, it is necessary to obtain a function to optimize. There are two functional of interest to the fuel management problem. The one is chosen when one wishes to obtain the maximum profit from operating power plant, and the other is chosen when one wishes to minimize the cost per unit energy of generating electricity.

The profit is equal to the dollars received for producing power less the cost of fuel burned and the interest charges for the fuel. The net grofit (NP) can be written as:

$$\mathbf{NP}=\int_0^T\int_{\text{vol}}\sum_i[(\mathbf{P}_i\sum_k\sigma_{ai}^k\phi^k-\mathbf{C}_i)\mathbf{N}_i]dxdt \quad (1)$$

where,

T : certain time,

$\mathbf{P}_i$: net income received from burning isotope i,

σ_{ai}^k: absorption cross section for isotope i in energy group k,

ϕ^k : neutron flux in energy group k,

$\mathbf{N}_i$: number density of isotope i,

$\mathbf{C}_i$: interest rate paid for isotope i.

To obtain a more compact notation, we will use an inner product form. The inner product notation for functions of a real variable is given by:

$$(f, g)=\int_0^x f(x)\, g(x)dx. \quad (2)$$

In Eq. (1), we see that we have an integration over two variables and a summation of $\sigma_{ai}^k\,\phi^k$ over k. This summation can be written as a dot product and if we consider our inner product to be an integration over two independent variables, we can rewrite Eq. (1) as:

$$(\mathbf{P}\sigma_a\cdot\phi-\mathbf{C}, \mathbf{N})=\int_0^T\int_{\text{vol}}\sum_i[(\mathbf{P}_i\sum_k\sigma_{ai}^k\phi^k-\mathbf{C}_i)\mathbf{N}_i]dxdt$$

where the quantities $\mathbf{P}, \mathbf{C}$, and $\mathbf{N}$ are vectors and the product includes the summation over these vectors.

There are several constraint equations which are to be applied to profit functional. These constraints are included by multiplying each constraint by a Lagrange multiplier and adding the result to the profit functional. This yields modified functional which is optimized by applying the variational method. The constraint equations which are included for this study consist of the group diffusion equations, the isotope burnup equations, and the inequality constraint equation on power peaking.

Let us study the burnup equations more closely. Any isotope of interest is produced either directly by fission, by decay from a precursor isotope, by neutron capture in the next lower isotope number or was there in the first place, thus:

$$\frac{d\mathbf{N}_i}{dt}=\lambda_{ji}\mathbf{N}_j+\sigma_{ai-1}\cdot\mathbf{N}_{i-1}-(\lambda_i+\sigma_{ai}\cdot\phi)\mathbf{N}_i+\gamma_i \quad (4)$$

where $\gamma_i = Y_{ij} N_j \sigma_{aj} \cdot \phi$ is the source equation for isotope i from direct fission yield. Y_{ij} means the partial fraction of isotope i. Eq. (4) can be written in matrix notations:

$$\frac{d\mathbf{N}}{dt} = \alpha\mathbf{N} + \gamma \tag{5}$$

where

N: nuclide number density vector,

α : nuclide net production matrix operator,

γ : nuclide source from fission vector. When the nuclide of interest, i, is a heavy isotope, γ_i is zero.

If we write $\beta = I\frac{d}{dt} - \alpha$, this becomes

$$\beta\mathbf{N} = \gamma. \tag{6}$$

Associated with the operator β is the adjoint operator β^+ defined by the relation

$$(\beta^+\mathbf{N}^+, \mathbf{N}) = (\mathbf{N}^+, \beta\mathbf{N}). \tag{7}$$

Consider the equqtion $\beta^+\mathbf{N}^+ = \gamma^+$ where, for the present, $\mathbf{N}^+$ and γ^+ are not given an interpretation. Now multiply Eq. (6) by $\mathbf{N}^+$, the adjoint equation by **N** and subtract gives:

$$(\mathbf{N}^+, \beta\mathbf{N}) - (\beta^+\mathbf{N}^+, \mathbf{N}) = (\mathbf{N}^+, \gamma) - (\gamma^+, \mathbf{N}). \tag{8}$$

The left hand side (LHS) of Eq. (8) is zero from the definition of β^+, thus:

$$(\mathbf{N}^+, \gamma) = (\gamma^+, \mathbf{N}). \tag{9}$$

Now to arrive at a meaning for γ^+ and $\mathbf{N}^+$, let us consider the functional $(\gamma^+, \mathbf{N})$ where γ^+ is arbitrary, and attempt to choose γ^+ in such a way that the functional is one of interest in a particular problem. The vector $\mathbf{N}^+$ is the adjoint number density, and if we wish to interpret it as an importance function, we must give $\mathbf{N}^+$ the units of a probability. Thus since $d\mathbf{N}^+/dt$ has the unit of inverse time, γ^+ must have the units of inverse time. As an example, suppose γ^+ is the reaction rate per nucleus in group k for the ith fission product at time t. Then

$$\gamma_i^+ = \sigma_{ai}^k \phi^k \delta(t-t'), \quad t' < T, \quad t < T \tag{10}$$

where $\delta(t-t')$ is the Dirac delta function.

Substituting Eq. (10) into RHS of Eq. (9) yields:

$$(\mathbf{N}_i^+, \gamma) = \int_0^T \int_{\text{vol}} \sigma_{ai} \cdot \phi \, \delta(t-t') \mathbf{N}_i(t') \, dx dt' = AB_i^k(t) \tag{11}$$

where $AB_i^k(t)$ is the absorption in fission product i in group k at time t. Thus $\mathbf{N}^+$ must be the importance of fission products of absorbing neutrons in energy group k at time t. Here we see that $\mathbf{N}^+(t')$ is the probability that a fission product source at t' yields an absorption reaction at a later time t. We now see that the sense of time for $\mathbf{N}^+$ and **N** is reversed. In the case of **N**, a source at t' yields the nuclide inventory given by **N** at all later times t. The adjoint number density $\mathbf{N}^+$ is considered to be an event at time t, in this case the absorption in group k, and to be the contribution of sources at all eadlier times. This arbitrariness of the source is important for it allows us to compare different problems for a property of interest without the necessity of solving the equations for each case.

Another adjoint source, γ^+, which could be considered is the decay energy produced at time t. In this case:

$$\gamma_i^+ = \lambda_i E_i \delta(t-t') \, \delta(x-x'), \; \begin{matrix} t<T, \; x<X \\ t'<T, \; x'<X \end{matrix} \tag{12}$$

where λ_i is the decay constant and E_i is the decay energy of nuclide i. From this

$$(\mathbf{N}^+, \gamma) = \int_0^T \int_{\text{vol}} \sum_i \lambda_i E_i \delta(t-t') \, \delta(x-x') \mathbf{N}_i(t') \, dx dt' = \int_{\text{vol}} \sum_i [\lambda_i E_i \mathbf{N}_i(t)] \, \delta(x-x') \, dx = E_T(x,t) \tag{13}$$

where the quantity $E_T(x,t)$ is the total decay energy at time t, and $\mathbf{N}_i^+(x,t)$ is the importance of a nuclide of type i for producing decay energy at time t and point X in the core.

The modified functional which is to be optimized can now be written as:

$$J = (\mathbf{P}\sigma_a \cdot \phi - \mathbf{C}, \mathbf{N}) - (\phi^+, \mathbf{L}\phi) - (\mathbf{N}^+, \beta\mathbf{N} - \gamma) - \{A, [1 - \mathbf{H}(x-A)][\sigma_a \cdot \phi\mathbf{N} - \mathbf{C}]\} \tag{14}$$

where

ϕ^+, $\mathbf{N}^+$, Λ: Lagrange multipliers,
$\mathbf{L}\phi=0$: matrix operator form of the group diffusion equations,
$\beta\mathbf{N}-\gamma=0$: matrix equation for the nuclide densities,
$\mathbf{H}(X-A)$: Heaviside operator,
A : transition point from the constraint region of the core to the unconstrained region,
t_1 : the time at which the region of the core from 0 to A is in the fully constrained state.

The form of the power constraint in Eq. (14) is chosen from the knowledge that the flux level is raised until the inequality constraint on the power density is satisfied. If the power level is to be raised even higher, there will be a region of the core which will operate at a constant power density, and this region of the core can be maintained at a constant power density only at time, t_1, during the core cycle.

It can be seen that variations of Eq. (14) with respect to ϕ and $\mathbf{N}$ will yield adjoint equations of the form:

$$(\gamma_\phi^+, \delta\phi)-(\mathbf{L}^+\phi^+, \delta\phi)=0, \tag{15}$$

$$(\gamma_N^+, \delta\mathbf{N})-(\beta^+\mathbf{N}^+, \delta\mathbf{N})=0. \tag{16}$$

Since the variations $\delta\phi$ and $\delta\mathbf{N}$ are arbitrary and independent, we have:

$$\gamma_\phi^+=\mathbf{L}^+\phi^+, \tag{17}$$

$$\gamma_N^+=\beta^+\mathbf{N}^+. \tag{18}$$

The units for ϕ^+ and $\mathbf{N}^+$ result from our choice of a profit functional. The profit is given in dollars, the quantity $\mathbf{L}\phi$ integrated over time and space has the units of neutrons: therefore, ϕ^+ has the units of dollars per neutron. The quantity $\beta_i\mathbf{N}_i$ integrated over space and time has the units of nuclear reactions in isotope i; therefore, $\mathbf{N}^+$ has the units of dollars per reaction in istope i.

For an example, we will assume only one burnable fuel isotope, and that all neutron absorptions in this isotope occur in the thermal group. All fission neutrons are assumed to be born in the fast group. The two group diffusion equations for this problem are:

$$D_1\nabla_2\phi_1+\nu\partial_f\mathbf{N}\phi_2-\Sigma_a'\phi_1=\frac{1}{v_1}\frac{\partial\phi_1}{\partial t}, \tag{19}$$

$$D_2\nabla^2\phi_2+\Sigma_R\phi_1-(\partial_a\mathbf{N}+\Sigma_a^2)\phi_2=\frac{1}{v_2}\frac{\partial\phi_2}{\partial t} \tag{20}$$

where Σ_a^1 and Σ_a^2 are the absorption cross sections for the nol-fuel isotopes in the core and the remainder of the notation is standard.

The burnup equation for the fuel is:

$$\frac{\partial\mathbf{N}}{\partial t}=-\sigma_a\phi_2\mathbf{N}. \tag{21}$$

The power constraint equation is:

$$\sigma_a\mathbf{N}\phi_2-\mathbf{C}^P\leq 0. \tag{22}$$

To maximize the profit for this problem it is necessary to raise the power level as high as possible. This leads us to the modified profit rate function given as:

$$J=(\mathbf{P}\sigma_a\phi_2-\mathbf{C}, \mathbf{N})-(\phi^+, \mathbf{L}\phi) - \{\Lambda, [1-\mathbf{H}(X-A)][\sigma_a\phi_2\mathbf{N}-\mathbf{C}^P]\}. \tag{23}$$

In order to find the optimizing equations, it is necessary to take variations of J with respect to $\mathbf{N}, \phi_1, \phi_2$, and A, also ϕ^+ and Λ but these do not lead to interesting results and therefore Eq. (23) must be written in explicit form:

$$\begin{aligned}J=&\int_0^T\int_0^X(\mathbf{P}\sigma_a\mathbf{N}\phi_2-\mathbf{C}, \mathbf{N})\,dXdt\\ &-\int_0^T\int_0^X\phi_1^+[D_1\nabla^2\phi_1+\nu\sigma_f\mathbf{N}\phi_2\\ &-\Sigma_a'\phi_1-\frac{1}{v_1}\frac{\partial\phi_1}{\partial t}]\,dXdt\\ &-\int_0^T\int_0^X\phi_2^+[D_2\nabla^2\phi_2+\Sigma_R\phi_1\\ &-(\sigma_a\mathbf{N}+\Sigma_a^2)\phi_2-\frac{1}{v_2}\frac{\partial\phi_2}{\partial t}]\,dXdt\\ &-\int_0^T\int_0^X\mathbf{N}^+\left[\frac{\partial\mathbf{N}}{\partial t}+\sigma_a\phi_2\mathbf{N}\right]dXdt\\ &-\int_0^T\int_0^X\wedge[1-\mathbf{H}(X-A)]\delta(t-t')(\sigma_a\mathbf{N}\phi_2\\ &-\mathbf{C}^P)\,dXdt\end{aligned} \tag{24}$$

where X is the outer dimension of the core.

The first equation is found by computing the variation of J with respect to N; thus

$$\begin{aligned}\delta J(\delta\mathbf{N}) &= 0\\ &= \int_0^T\int_0^X (\mathbf{P}\sigma_a\phi_2 - \mathbf{C})\delta\mathbf{N}dXdt\\ &- \int_0^T\int_0^X (\nu\sigma_f\phi_1^+ - \sigma_a\phi_2^+)\phi_2\delta\mathbf{N}dXdt\\ &+ \int_0^T\int_0^X \left[\frac{\partial\mathbf{N}^+}{\partial t} - \sigma_a\phi_2\mathbf{N}^+\right]\delta\mathbf{N}dXdt\\ &- \int_0^X [\mathbf{N}^+\delta\mathbf{N}|_0^T]dX\\ &- \int_0^T\int_0^X \wedge[1-\mathbf{H}(X-A)]\delta(t-t_1)\sigma_a\phi_2\delta\mathbf{N}dXdt. \end{aligned} \quad (25)$$

Since this equation must be true for arbitrary variations of $\delta\mathbf{N}$, we obtain:

$$\mathbf{P}\sigma_a\phi_2 - \mathbf{C} - (\nu\sigma_f\phi_1^+ - \sigma_a\phi_2^+)\phi_2 + \frac{\partial\mathbf{N}^+}{\partial t} - \sigma_a\phi_2\mathbf{N}^+ - \wedge[1-\mathbf{H}(X-A)]\sigma_a\phi_2\delta(t-t_1) = 0 \quad (26)$$

$$\int_0^X [\mathbf{N}^+(T)\delta\mathbf{N}(T) - \mathbf{N}^+(0)\delta\mathbf{N}(0)]dX = 0. \quad (27)$$

The term $\nu\sigma_f\phi_1^+ - \sigma_a\phi_2^+$ is the net neutron importance of an interaction in fuel The term $\Lambda[1-\mathbf{H}(X-A)]\sigma_a$ is the penalty one must pay for designing the reactor for a flat power distribution.

If Eq. (26) is integrated over space and time, and the condition Eq. (27) is applied, we get

$$\begin{aligned}&\int_0^T\int_0^X (\mathbf{P}\sigma_a\phi_2 - \mathbf{C})dXdt\\ &= \int_0^T\int_0^X (\nu\sigma_f\phi_1^+ - \sigma_a\phi_2^+)\phi_2 dXdt\\ &+ \int_0^T\int_0^X \sigma_a\phi_2\mathbf{N}^+dXdt\\ &+ \int_0^X \Lambda[1-\mathbf{H}(X-A)]\sigma_a\phi_2(X,t_1)dt. \end{aligned} \quad (28)$$

This equation implies that the average profit is equal to the net value of neutrons per unit volume plus the value of neutron reactions per unit volume plus the cost of maintaining flat power per unit volume, all on a per atom basis. This interpretation is a direct result of Eq. (27) and is in the form of a cost balance.

If the inner product of Eq. (26) is taken with N and the direct number density equation is inner multiplied by $\mathbf{N}^+$ and added to Eq. (26), we obtain

$$\begin{aligned}(\mathbf{P}\sigma_a\phi_2 - \mathbf{C}, \mathbf{N}) &= (\nu\sigma_f\phi_1^+ - \sigma_a\phi_2^+, \phi_2\mathbf{N})\\ &+ \int_0^X [\mathbf{N}^+(X,0)\mathbf{N}(X,0)\\ &- \mathbf{N}^+(X,T)\mathbf{N}(X,T)]dX\\ &+ \{\Lambda[1-\mathbf{H}(X-A)]\sigma_a, \phi_2\mathbf{N}\delta(t-t_1)\}. \end{aligned} \quad (29)$$

Eq. (29) implies that the net profit is equal to the net value of neutrons plus the change in value of the fuel plus the cost of achieving flat power over a region of the reactor at time t_1.

Variations with respect to ϕ_1 and ϕ_2 are taken in the same manner and yield the following differential equations and initial final value conditions:

$$D_1\nabla^2\phi_1^+ + \Sigma_R\phi_2^+ - \Sigma_a^1\phi_1 = -\frac{1}{v_1}\frac{\partial\phi_1^+}{\partial t}, \quad (30)$$

$$D_2\nabla^2\phi_2^+ + \nu\sigma_f\mathbf{N}\phi_1^+ - (\sigma_a\mathbf{N} + \Sigma_a^2)\phi_2^+ = -\frac{1}{v_2}\frac{\partial\phi_2^+}{\partial t} - \mathbf{P}\sigma_a\mathbf{N} + \sigma_a\mathbf{N}\mathbf{N}^+ + \Lambda\sigma_a\mathbf{N}, \quad (31)$$

$$\int_0^X [\phi_1^+(X,T)\delta\phi_1(X,T) - \phi_1^+(X,0)\delta\phi_1(X,0)]dX = 0, \quad (32)$$

$$\int_0^X [\phi_2^+(X,T)\delta\phi_2(X,T) - \phi_2^+(X,0)\delta\phi_2(X,0)]dX = 0. \quad (32)$$

If Eq. (30) is multiplied by ϕ_1 and added to Eq. (31) multiplid by ϕ_2, and the resultant equation is subtracted from the corresponding group diffusion equations multiplied by ϕ_1^+ and ϕ_2^+, we get:

$$(\mathbf{P}\sigma_a\phi_2, \mathbf{N}) = (\sigma_a\mathbf{N}\phi_2, \mathbf{N}^+) \quad (34)$$

Eq. (34) implies that the gross profit from neutron interactions in $\mathbf{N}$ is equal to the value of burning isotope $\mathbf{N}$. These adjoint equations which result from variations with respect to $\mathbf{N}$, ϕ_1, and ϕ_2 have interesting physical interpretations.

The equations which are necessary are derived by computing the variation of the profit functional with A and t_1. It will be recalled that when the variation of A was computed, all contributions from the constraint equations were zero. This also occurs when we take the variation with respect to t_1 and leaves:

$$\int_0^T\int_0^X \left[\mathbf{P}\sigma_a \frac{\partial(\phi_2\mathbf{N})}{\partial t_1} - C\frac{\partial \mathbf{N}}{\partial t_1} \right] dX\,dt=0. \tag{35}$$

The variation with respect to A yields:

$$\int_0^T\int_0^X \left[\mathbf{P}\sigma_a \frac{\partial(\phi_2\mathbf{N})}{\partial A} - C\frac{\partial \mathbf{N}}{\partial A} \right] dX\,dt=0. \tag{36}$$

Eqs. (35) and (36) are solved in conjunction with the group diffusion equations and the constraint equations to yield the optimum time t_1 and flat power dimension A. Since these equations are implicit for t_1 and A, we need non-linear methods to compute the optimum.

III. The Search Method

Some type of non-linear search method was required to solve for the optimum enrichments. Since it is necessary to apply search methods to locate the optimum enrichments, even when the equations for the cost function are solved explicitly, it is just as practical to solve the cost function equation and constraint equations numerically and use modern optimization procedure to locate the optimum.

The search method proceeds in three stages: (1) compute the cost gradient, (2) search for the optimum distance in the gradient direction, and (3) after gradient procedures net no further gain, end the calculation with a Newton-Raphson search.

A. The Method of Gradient

The following derivation closely follows the work of Wilde and Beightler[8]. The fuel cycle cost (CS) can be written as a function of the three enrichments, thus

$$\mathrm{CS}=f(e_1, e_2, e_3). \tag{37}$$

The gradient of the cost about e_1, e_2, and e_3 can be computed by computing the cost of perturbations of these enrichments and using the results in

$$\frac{\partial \mathrm{CS}}{\partial e_1}=\frac{f(e_1+\delta e_1, e_2, e_3)-f(e_1-\delta e_1, e_2, e_3)}{\partial \delta e_1},$$
$$\frac{\partial \mathrm{CS}}{\partial e_2}=\frac{f(e_1, e_2+\delta e_2, e_3)-f(e_1, e_2-\delta e_2, e_3)}{\partial \delta e_2},$$
$$\frac{\partial \mathrm{CS}}{\partial e_3}=\frac{f(e_1, e_2, e_3+\delta e_3)-f(e_1, e_2, e_3-\delta e_3)}{\partial \delta e_3}. \tag{38}$$

The gradient of the cost function can now be written as

$$\nabla \mathrm{CS}=\frac{\partial \mathrm{CS}}{\partial e_1}\hat{e}_1+\frac{\partial \mathrm{CS}}{\partial e_2}\hat{e}_2+\frac{\partial \mathrm{CS}}{\partial e_3}\hat{e}_3. \tag{39}$$

Let us now consider a small sphere and compute the point on the sphere

$$|d\vec{e}\,|^2 r^2 \tag{40}$$

which gives us the maximum change in fuel cycle cost. To affect this, we scalar multiply Eq. (39) by the enrichment vector, and to this the constrain Eq. (40) multiplied by the Lagrange multiplier, λ, gives

$$\Delta \mathrm{CS}=\nabla \mathrm{CS}\cdot d\vec{e}+\lambda[\,|d\vec{e}\,|^2-r^2]. \tag{41}$$

Differentiating Eq. (41) with respect to the enrichment vector gives

$$\nabla \mathrm{CS}+2\lambda d\vec{e}=0 \tag{42}$$

From Eq. (42) it can be seen that since λ is a constant, the optimum enrichment vector must point along the gradient vector. Solving Eq. (42) for the differential enrichment vector, and substituting this result into Eq. (40), yield the value of λ

$$\lambda=\pm\frac{1}{2r}|\nabla \mathrm{CS}|. \tag{43}$$

This value of λ substituted back into Eq. (42) gives us the value of the enrichment

$$d\vec{e}=\pm\frac{r}{|\nabla \mathrm{CS}|}\nabla \mathrm{CS}. \tag{44}$$

Note that Eq. (44) contains a plus and minus sign in front of the gradient; this says that the maximum increase in fuel cycle cost is found by traveling in the positive gradient direction

to the sphere and the maximum decrease in fuel cycle cost is found by traveling in the nagative gradient direction to the sphere.

Now that it is known in what direction to travel to seek minimum fuel cycle cost, it is necessary to learn how far to travel in this direction before no further improvement is made.

B. The Section Search

It is shown in Wilde and Beightler that a Fibbonacci[9] search is most efficient over a known region with a known number of trials allowed to reduce the region of search. In this search, however, the number of trials is not known; therefore, the golden-section search is used to compute trials to reduce the search region size.

Let us suppose we are searching over a uninodal function such as shown in Figure 1. If the cost is evaluated at 0 and 1, and two calculations are performed within this region, a and b, the region between b and 1 can be eliminated from the search domain. This conclusion can be reached because the search is over a uninodal function and therefore since

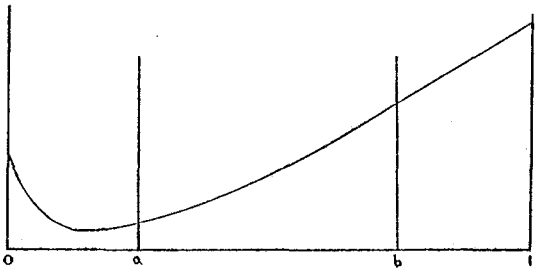

Fig. 1. Uninodal Function

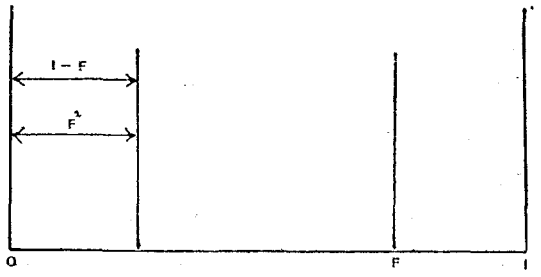

Fig. 2. Golden Section Search

the cost at a is less than the cost at b, the region to the right of b can be eliminated. Another point can be computed within the region zero to b and by comparing costs, a still smaller search domain can be established.

Let us now choose our points a and b symmetrically in the search region such that when an elimination of part of the search region is made, the remainning section is the same fraction of the samller region as the other point did for the large region, as shown in Figure 2. This leads us to

$$f^2=1-f \tag{45}$$

The only positive root satisfying Eq. (45) is $f=0.618$. This value of f rapidly reduces the size of the search domain as shown in Table 1.

Table 1. Golden Section Convergence

Trials	Cases	Total cases	Region remaining
1	2	2	0.618
2	1	3	$(0.618)^2$
3	1	4	$(0.618)^3$
⋮	⋮	⋮	⋮
N	1	$N+1$	$(0.618)^N$

For this study it was found that a search region which changed any enrichment by a maximum of 0.2 w/o U-235 from the base calculation always included the optimum distance along the gradient direction. Once this optimum distance was found a new gradient was computed about this optimum and the search was continued. After a few gradient searches were carried out, it was found that the optimum could not be improved.

C. The Newton-Raphson Method

A Newton-Raphson extrapolation was used to find the "true" optimum enrichments. This method of optimum seeking consists of expanding the cost function in the second order Taylor series form

$$CS(e_1, e_2, e_3)=CS(e_1^0, e_2^0, e_3^0)$$
$$+a(e_1-e_1^0)+b(e_2-e_2^0)+c(e_3-e_3^0)$$

$$+a'(e_1-e_1^0)^2+b'(e_2-e_2^0)^2+c'(e_3-e_3^0)^2$$
$$+a''(e_1-e_1^0)(e_2-e_2^0)+b''(e_1-e_1^0)(e_3-e_3^0)$$
$$+c''(e_2-e_2^0)(e_3-e_3^0) \quad (46)$$

where:

$$a=\frac{\partial CS}{\partial e_1}\Big|_{e_1^0,\,e_2^0,\,e_3^0}, \quad b=\frac{\partial CS}{\partial e_2}\Big|_{e_1^0,\,e_2^0,\,e_3^0},$$
$$c=\frac{\partial CS}{\partial e_3}\Big|_{e_1^0,\,e_2^0,\,e_3^0}, \quad a'=\frac{1\partial^2 CS}{2\partial^2 {e_1}^2}\Big|_{e_1^0,\,e_2^0,\,e_3^0},$$
$$b'=\frac{1\partial^2 CS}{2\partial^2 {e_2}^2}\Big|_{e_1^0,\,e_2^0,\,e_3^0}, \quad c'=\frac{1\partial^2 CS}{2\partial^2 {e_3}^2}\Big|_{e_1^0,\,e_2^0,\,e_3^0},$$
$$a''=\frac{\partial^2 CS}{\partial e_1\partial e_2}\Big|_{e_1^0,\,e_2^0,\,e_3^0}, \quad b''=\frac{\partial^2 CS}{\partial e_1\partial e_3}\Big|_{e_1^0,\,e_2^0,\,e_3^0},$$
$$c''=\frac{\partial^2 CS}{\partial e_2\partial ee}\Big|_{e_1^0,\,e_2^0,\,e_3^0}.$$

The constants of Eq. (46) can be evaluated by computing the cost at ten points in the vicinity of e_1^0, e_2^0, and e_3^0. The partial derivatives of Eq. (46) with respect to each of the enrichments can then be set to zero and the resulting equation can be evaluated to give the true optimum.

The matrix form of the equations which are obtained by setting the partial derivatives with respect to the enrichments to zero given by

$$[\mathbf{A}][\Delta\hat{e}]=-[\mathbf{D}] \text{ or } [\Delta\hat{e}]=-[\mathbf{A}]^{-}[\mathbf{D}] \quad (47)$$

where:

$$[\Delta\hat{e}]^T=[e_1-e_1^0 \;\; e_2-e_2^0 \;\; e_3-e_3^0]$$
$$[\mathbf{D}]^T=\left[\frac{\partial CS}{\partial e_1} \;\; \frac{\partial CS}{\partial e_2} \;\; \frac{\partial CS}{\partial e_3}\right]$$
$$[\mathbf{A}]=\begin{pmatrix} \frac{\partial^2 CS}{\partial^2 {e_1}^2} & \frac{\partial^2 CS}{\partial e_1\partial {e_2}^2} & \frac{\partial^2 CS}{\partial e_2\partial {e_3}^2} \\ \frac{\partial^2 CS}{\partial e_1\partial e_2} & \frac{\partial^2 CS}{\partial^2 e_2} & \frac{\partial^2 CS}{\partial e_2\partial e_3} \\ \frac{\partial^2 CS}{\partial e_1\partial e_3} & \frac{\partial^2 CS}{\partial e_2\partial e_3} & \frac{\partial^2 CS}{\partial^2 e_3} \end{pmatrix}$$

The solution, Eq. (47), is the Newton-Raphson equation for the extrapolation to the optimum enrichments e_1, e_2, and e_3.

IV. Computational Model and Computational Results

The optimization procedure described in Ⅲ was used to locate the optimum enrichments for two different fuel management schemes: (1) a three region batch loaded reactor and (2) a three region out-in cycled reactor. The cost function for both schemes is identical because no attempt was made to include the cost of refueling the reactor.

The reactor which was designed had the cell dimensions and uranium loading of a typical pressurized water reactor with water to metal ratio of 4.2. Two group microscopic cross sections were obtained from the mit-life of a Westinghouse LEOPARD[10] calculation for 2.7 w/o U-235. The fast to thermal flux ratio from this case was used to develop one group microscopic cross sections. These one group cross sections were used for all the calculatons described below.

The reactor was calculated as a slab reactor with three equal volume regions each 27cm thick. A 9cm thick water reflector was added to the outer region.

The finite difference calculation was performed using the one dimensional diffusion code MAIDS[11]. Burnup calculations were performed region-wise in 2000 hour time steps. Equilibrium Xe-135 and Sm-149 was assumed at all time steps, and the production of heavy isotopes was computed for U-235, U-236, U-238, Pu-239, Pu-240, Pu-241, and Pu-242. The gross fission products were assumed to burn linearly with time.

In order to properly incorporate the power peaking factor into the cost function, it was necessary to carry out the calculations such that the peak power density was achieved at all times throughout the core life. At each time step a search was performed to locate the peak power density and all fluxes were normalized to this peak power density. The peak power density that was used was 100 watts/cm^3 for all cases. Since the reactor was assumed to be

a cube 132cm on a side, this yielded a maximum thermal power of 425 MW.

The end of core life inventories were computed by interpolating between two successive k's, one greater than 1.0 and one less than 1.0, to an effective k of 1.0. Inventories from this end of life case were then inserted into the cost code to compute the fuel cycle cost. The net fuel cycle cost was found by computing the cost for each region and then weighting this cost by the energy produced from the region.

Four complete cycles of core operation were computed for each case of the cycled reactor. The reactor was cycled from the outer most region to the inner most with fuel from the central zone being discharged from the reactor. The eorichment which was assumed to become the equilibrium cycle enrichment was fed at the beginning of the second cycle and this same enrichment was fed for both the third and fourth cycles. As the two outer regions of the fourth cycle had only been in the reactor for one and two cycles. respectively, the appropriate increment of burnup, as computed during the fourth cycle, was added to these regions to yield an effective three cycle burnup on these regions.

A. Batch Reactor

Table 2 gives a summary of the approach to the optimum reactor. Each different gradient direction is given as a step number, and the distance along that gradient direction from the preceding step is labeled R. Step zero is the obtimum one enrichment reactor which was obtained by a golden section search in the enrichment range zero to five weight per cent. In the past it has been common practice to correlate the obtimum fuel distribution with the optimum power distribution at the beginning of core life. For this reason Table 2 also includes the ratio of the maximum power in the reactor to the average power, P_{max}/P_{av}.

Although the optimum reactor has the best

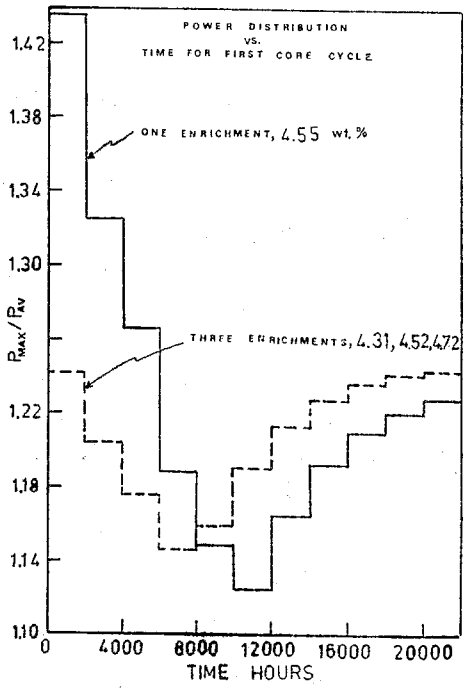

Fig. 3. First Cycle Power Distribution for a Batch Reactor

Table 2. Batch Reactor Calculations

Step No.	R	Average Cost mills/Kwh	P_{max}/P_{av}	Enrichment, w/o		
				e_1	e_2	e_3
0	—	1.87751	1.4371	4.55	4.55	4.55
1	0.2	1.87267	1.2874	4.39	4.66	4.61
2	0.09	1.87196	1.2998	4.41	4.59	4.66
3	0.0474	1.87142	1.2646	4.37	4.60	4.68
4	0.0382	1.87126	1.2625	4.36	4.57	4.70
5	Newton-Raphson	1.87094	1.2420	4.31	4.52	4.70

power distribution the improvement in cost in moving from step 1 to step 2 is accompanied by a decrease in power capability at the beginning of core life. Thus one should be reluctant to optimize a reactor only from beginning of life power capability considerations.

The comparison of power distribution at the beginning of core life is a superficial comparison, for the power distribution changes with burnup. In Figure 3 we plot curves of the power capability as a function of time for the optimum three enrichment reactor. Here we see that the power capability increases for a while with burnup, but then decreases toward the end of core life. Indeed for the obtimum three enrichment reactor, the power distribution is the poorest at the end of core life by a very narrow margin.

We also see from Table 2 that our optimization procedure continually moves in the direction of decreased cost, and that the final application of the Newton-Raphson procedure does yield the lowest fuel cycle cost. The optimum three enrichment reactor shows very little improvement in cost, 0.006mills/Kwh, over the optimum one enrichment reactor.

Table 3. Cycle Reactor Calculations

Step No.	R	Average Cost mills/Kwh	Enrichment, w/0 e_1	e_2	e_3	e_4
0	—	1.70983	3.26	3.26	3.26	3.26
1	0.3	1.70298	3.20	3.36	3.39	3.02
2	0.2	1.69975	3.18	3.35	3.55	3.14
3	0.1	1.69886	3.22	3.35	3.59	3.06
4	0.1*	1.69754	3.25	3.40	3.63	3.13
5	0.2	1.69576	3.36	3.50	3.73	3.04
6	0.05	1.69499	3.37	3.51	3.74	3.09
7	**	1.69441	3.47	3.61	3.74	3.09
8	**	1.69418	3.47	3.61	3.84	3.09

*Beginning with this step number all gradient were computed using central differencing. Prior to this point the gradient was computed by forward differencing.

**The last two step numbers were obtained while computing cross-derivatives for the Newton-Raphson method.

B. Cycled Core

In Table 3 a summary of the cycled core calculation is presented. Again the step numbers refer to different gradient directions with step zero corresponding to a golden section search performed for one enrichment. The optimum normalized distance along the gradient direction is given as R.

A result of Table 3 shows that there is little net improvement in fuel cycle cost as we move from the optimum one enrichment case to the best four enrichment case, 0.015 mills/Kwh.

We also notice that the enrichment for the first core in the optimum four enrichment case are higher than the equilibrium cycle enrichment, e_4. This result is unusual in fuel cycle studies in that the first core of pressurized water reactor is designed for lower enrichments than the equilibrium enrichment. By using enrichments in the first core, one increases the first core cycle time and burnup thereby par-

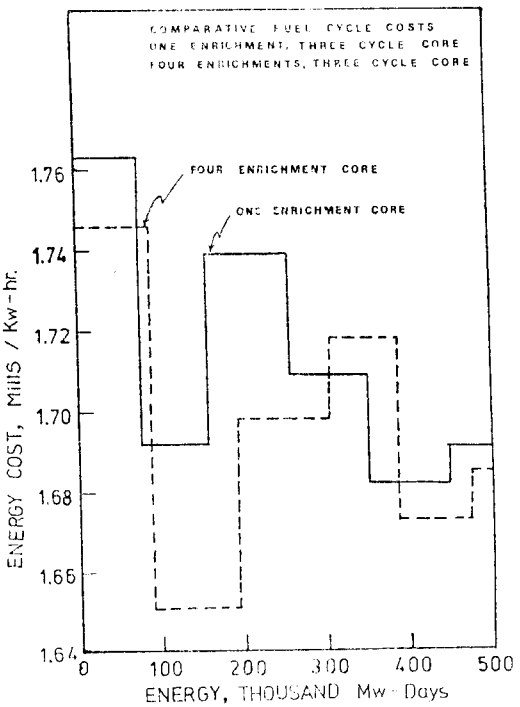

Fig. 4. Comparative Fuel Cycle Cost for a Cycled Core

Table 4. Power Ratios for a Cycled Reactor

Step No.	R	Averge Cost mills/Kwh	Ratio of P_{max}/P_{av}			
			cycle 1	cycle 2	cycle 3	cycle 4
0	—	1.70983	1.4371	1.5750	1.5472	1.5166
1	0.3	1.70298	1.2841	1.3916	1.4022	1.3615
2	0.2	1.69975	1.2283	1.4754	1.4068	1.4366
3	0.1	1.69886	1.2322	1.4173	1.4221	1.3853
4	0.1	1.69754	1.2225	1.4652	1.4645	1.4393
5	0.2	1.69576	1.2357	1.4192	1.4082	1.3711
6	0.05	1.69499	1.2363	1.4313	1.4385	1.4029
7	*	1.69441	1.2771	1.4288	1.4386	1.4026
8	*	1.69418	1.2417	1.4373	1.4373	1.4018

* Results of Newton-Raphson cross-derivatives.

tially eliminating the penalty one usually obtains for discharging a partially burned region of fuel.

Figure 4 is a curve of the region-wise fuel cycle cost as a function of the net thermal energy produced. In this figure, each region is represented by an ordinate of constant value and the distance along the abscissa represents the thermal energy produced. From this curve it is seen that there be still a penalty for discharging the partially irradiated first region of fuel; however, this penalty is compensated by the improvement in cost in the highly irradiated regions two and three.

It is again interesting to see if there is any correlation of the beginning of cycle power distribution with the fuel cycle cost. Table 4 shous the ratio of P_{max}/P_{av} with the gradient direction and fuel cycle cost.

We can see from Table 4 that each of the beginning-of-cycle power distributions for step 4 is better than the corresponding power distribution for step 9, and that the average fuel cycle cost for step 9 is 0.004 mills/Kwh lower than for step 4. Thus we again conclude that there is no simple correlation of optimum fuel cycle cost with power distribution.

We finally observe that the absolute optimum for the cycled core study was not obtained. The Newton-Raphson calculations was carried out for steps 6 and 7. For the both cases the method moved the optimum far from the base point, and the fuel cycle cost for cross-derivative calculations proved to be lower than the costs computed from extrapolation.

Since the expense of carrying out the cycled core calculations were prohibitive, it was impossible to pursue them to a satisfactory conclusion. It is noted, however, that when the Newton-Raphson calculation was performed for the batch reactor, the apparent optimum, the optimum obtained by the gradient method yielded a lower fuel cycle cost than any of the perturbations which were introduced to compute the cross derivatives. Therefore, the Newton-Raphson calculation for the batch reactor was actually an interpolation for the optimum.

V. Conclusions

The variational problem which was studied in this investigation demonstrated the relationship which exists between reactor fuel inventory and power capability. It also demonstrated the power manner in which to handle inequality constraints which arises in fuel management studies. Finally we found that the Lagrange multipliers which are used to handle constraint

problems are actually importance functions deriving their exact interpretation from the functional to be optimized.

Trial functions for the fuel distribution consisting of a constant fuel loading in each region of a three equal volume region reactor were used in conjunction with the equality constraints of the heavy isotope burnup equations and an inequality constraint on the maximum allowable power density, to minimize the fuel cycle cost of a typical batch and cycle loaded pressurized water reactor. It is that this could be optimized using standard optimization procedures, the method of gradients and Newton-Raphson interpolation.

In this study we find that there is little improvement in fuel cycle cost, within the framework of a given fuel management when the region enrichments are varied. This is partially because the plant capital charges are not included in our cost function. It also indicates that fuel cycle economics are more readily improved by: (1) improving core performance, designing the core to operate at higher allowable power densities, and (2) changing the possibilty of using the concept of "fuel sharing".

The physical model and the economic model which were used for this study are quite simple; a one-group slab reactor with region-wise fuel depletion and did not incorporate refueling costs, plant capital charges or a constraint on annuual refueling.

It must be noted, however, that the inclusion of a more complicated physics or economics model does not alter the optimization procedure. The procedure which is described would be particularly useful to optimize a very detailed model of a reaactor in which the fuel remains stationary during its core resident time, such as a roundelay fueled reactor.

The variatioal approach which is used herein is quite general and can be applied to many reactor problems. The drimary concern for ane engineer using this procedure is to be certain that the functional being optimized is actually the functional of physical importance to the problem at hand.

Acknowledgement

I wish to express my sincere gratitude to Professor, Charles W. Maynard, Nuclear Engineering Department, University of Wisconsin-Madison, for many fruitful discussions on the concepts and particularly for his help in clarifying the role of adjoint function which arise in constrained variational problems.

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