USE OF GENERALIZED PERTURBATION METHODS FOR OPTIMIZATION OF REACTOR DESIGN*

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Abstract—A method is described which adopts the generalized perturbation theory and programming techniques for optimizing reactor integral parameters, linear or bilinear in the real and adjoint neutron fluxes, after assumption of given constraints.

An application of this method to the optimization of the beryllium distribution, with respect to the Doppler effect in a fast ceramic test reactor, is illustrated.

1. INTRODUCTION

The availability of fast computers of increasingly higher performance suggests the development of more and more sophisticated techniques for the optimization of power reactor design. In the present paper an optimization method is described regarding a specific reactor problem. However, the optimization procedure suggested may easily be extended to a number of cases of interest relevant to control, economics, safety.

The specific problem considered deals with the need of ensuring an intrinsic safety mechanism in a 500 l. ceramic fast test reactor fuelled with $^{235}$U enriched uranium and cooled with sodium. For this purpose it has been deemed convenient to find the optimal distribution of a given quantity of beryllium oxide in the four subregions into which the driver core surrounding the test region has been subdivided, so that the Doppler reactivity effect is enhanced. This is consequent to the increase of the neutron flux at low energies where the capture resonances of $^{238}$U are present. Therefore, a prompt negative feedback is ensured in case of an accidental excursion leading to a temperature increase. In the present analysis a temperature increase $\Delta T$ of 1200°C, starting from operating conditions, has been assumed.

The method developed for this specific purpose allows us to calculate the optimal beryllium distribution, certain limiting conditions, or constraints, being given. Once these constraints and the quantity to be optimized are set, the basic procedure consists in the linearization of the problem which is properly allowed for through the use of the generalized perturbation techniques (Gandini, 1967). By means of these techniques it is possible to relate linearly the change of a given material density (or of a cross section) to ratios of quantities, linear or bilinear in the real and adjoint neutron fluxes, such as the Doppler reactivity effect. The standard programming techniques may then be applied.

2. CONDITIONS ASSUMED

Let us represent the Doppler reactivity effect consequent on a core temperature change $\Delta T$ by the functional (using a multigroup vector notation):

$$
\rho_{ED} = \frac{\int_{\text{syst}} \varphi * \Delta \varphi \, \text{d}r}{\int_{\text{syst}} \varphi * F\varphi \, \text{d}r}
$$

(1)

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where $\Delta P$ represents the perturbation of the Boltzmann operator $P$ related to the temperature change $\Delta T$ and $F$ represents the fission neutron source matrix. The vector functions $\varphi$ and $\varphi^*$ represent the multigroup real and adjoint neutron fluxes.

Our problem consists in redistributing a given amount of beryllium oxide, or in distributing larger amounts, in the driver region, so that the negative Doppler effect reaches a maximum in absolute value. The composition of the centred test region is kept fixed. These beryllium distributions must satisfy a number of constraints and technological specifications:

1. The reactor must be maintained critical by changing its $^{235}\text{U}$ enrichment which must be the same in all subregions.
2. The power of the test region is fixed.
3. The power in each fuel pin must not be higher than a safety limit.
4. The sum of the beryllium oxide volume fraction and that of the fuel, in each concentric subregion into which the driver core is subdivided, must be kept constant.
5. The amount of beryllium oxide to be distributed is fixed.

3. DESCRIPTION OF THE METHOD

The model assumed for the calculation is represented by a fast driver core subdivided into $N$ subregions corresponding to the rows of the fuel subassemblies.

We then assume that in each driver subregion $n$ the material replacements are relevant to $M$ materials (e.g. $^{235}\text{UO}_2$, $^{238}\text{UO}_2$, BeO).

The optimization of $\rho_{\text{ED}}$ also corresponds to the maximization of the fractional quantity:

$$
\frac{\delta \rho_{\text{ED}}}{\rho_{\text{ED}}} = \sum_{n=1}^{N} \sum_{m=1}^{M} a_{n,m} x_{n,m} 
$$

where $x_{n,m}$ represents (in weight) the amount of material $m$ introduced into, or subtracted from region $n$. The coefficients $a_{n,m}$ are sensitivity coefficients calculable by means of generalized perturbation formulae. The coefficients $a_{n,m}$ relative to the materials involved in the operator $\Delta P$ of equation (1) are the sum of two contributions: one related to an indirect effect (spectral effect), the other one related to a direct effect (material density change).

The restrictive conditions mentioned above may be translated into quantitative relations as shown below.

(a) Criticality condition

It is necessary that the criticality of the system is not affected by the optimization. We then consider the ratio:

$$
\rho_{\text{Mat}} = \frac{\int_{\text{syst}} \varphi^* P \varphi \ dr}{\int_{\text{syst}} \varphi^* F \varphi \ dr}
$$

where $\sigma$ is the Boltzmann operator related to the material distribution in the reactor.
Use of generalized perturbation methods for optimization of reactor design

Recalling that $P\Phi = 0$ for a critical system, $\rho_{\text{Mat}} = 0$. The criticality condition becomes:

$$\delta \rho_{\text{Mat}} = \sum_{n=1}^{N} \sum_{m=1}^{M} b_{n,m} x_{n,m} = 0$$  \hspace{1cm} (4)

where the coefficients $b_{n,m}$ may be calculated using the conventional perturbation techniques.

(b) **Constant enrichment condition**

The enrichment must be constant in all the driver subregions. If $m_1$ is the fissile material index and $m_2$ that of the fertile one, this condition may be represented by the quadratic equations:

$$\frac{x_{N,m_1} + x_{N,m_2}}{x_{N,m_2} + x_{N,m_1}} = \frac{x_{n,m_1} + x_{n,m_2}}{x_{n,m_2} + x_{n,m_1}} \quad [n = 1, 2, \ldots, (N - 1)]$$  \hspace{1cm} (5)

where $x_{n,m}$ represents the amount of material $m$ in region $n$ before the optimization. The $N$-th (i.e. outer) subregion has optionally been chosen as a reference. We shall linearize equation (5) considering $x$ a second order quantity with respect to $\tilde{x}$ and disregarding third order terms. We obtain:

$$\tilde{x}_{N,m_1} x_{n,m_1} + \tilde{x}_{N,m_2} x_{n,m_2} + \tilde{x}_{N,m_1} x_{n,m_2} + \tilde{x}_{N,m_2} x_{n,m_1} = \tilde{x}_{n,m_1} \tilde{x}_{n,m_1} - \tilde{x}_{N,m_2} \tilde{x}_{n,m_1} \quad [n = 1, 2, \ldots, (N - 1)].$$  \hspace{1cm} (6)

(c) **Pin power limit condition**

If the integrated power $Q_{\text{test}}$ of the test region is fixed, we may write:

$$Q_{\text{test}} = q \int_{\text{test}} \Phi' \sum_{f}^{\text{test}} \mathrm{d}r = K_{\text{test}}$$  \hspace{1cm} (7)

where $K_{\text{test}}$ is a given positive constant, $q$ represents the energy per fission, and $\Phi'$ the neutron flux perturbed by the material redistribution due to the optimization process. On the other hand, in each subregion $n$ the power per fuel pin $Q_n$ must be limited for safety reasons. Therefore, it must be:

$$Q_n = q \sum_{i=1}^{\Phi} \gamma_n (\tilde{x}_{n,m_1} + x_{n,m_1}) \alpha_m \mathrm{d}r$$

$$\times \frac{x_{n,m_1} + x_{n,m_2}}{\alpha_n [x_{n,m_1} + x_{n,m_1} + (x_{n,m_2} + x_{n,m_2})]} \leq K_0$$  \hspace{1cm} (8)

where $K_0$ is another given positive constant, $\gamma_n$ is a coefficient which translates the weights ($\tilde{x}$ - $x$) relative to the fissile and fertile materials into volume fractions and $\alpha_n$ represents the number of fuel pins in the $n$-th region in the system before the optimization. Therefore, the fractional coefficient in (8) represents the inverse of the number of the fuel pins after the optimization.

Our condition may now be written:

$$\frac{Q_n}{Q_{\text{test}}} \leq \frac{K_0}{K_{\text{test}}} = \mathcal{K} \quad (n = 1, 2, \ldots, N).$$  \hspace{1cm} (9)
Recalling expressions (7) and (8) and that the quantities \( \bar{x}_{n,m} + x_{n,m} \) are assumed to be always positive, condition (9) becomes:

\[
\sum_{i=1}^{2} (\bar{x}_{n,m_i} + x_{n,m_i}) \rho'_{n,i} = \frac{\hat{K} \alpha_n (\bar{x}_{n,m_1} + x_{n,m_1}) + (\bar{x}_{n,m_2} + x_{n,m_2})}{\gamma_n (\bar{x}_{n,m_1} + \bar{x}_{n,m_2})} \leq 0
\] (10)

where

\[
\rho'_{n,i} = \int_{\Gamma(n)} \varphi' \varphi'_{n,m_i} \, dr \quad (i = 1, 2).
\] (11)

The difference \( \delta \rho_{n,i} \) between the perturbed values \( \rho'_{n,i} \) and the unperturbed ones \( \rho_{n,i} \) may also be written in terms of the generalized perturbation techniques. Limiting the approximation to first order, we may write the following fractional variations:

\[
\frac{\delta \rho_{n,i}}{\rho_{n,i}} = \sum_{n=1}^{N} \sum_{m=1}^{M} c_{u,m}^{(n,i)} x_{u,m} \quad (i = 1, 2)
\] (12)

where \( c_{u,m}^{(n,i)} \) are calculable coefficients relative only to indirect (i.e. spectral) effects on functionals \( \rho_{n,i} \). Substituting in (10) \( \rho'_{n,i} \) with \( \rho_{n,i} + \delta \rho_{n,i} \) and recalling expressions (12) for \( \delta \rho_{n,i} \) we obtain:

\[
\sum_{i=1}^{2} \rho_{n,i} (\bar{x}_{n,m_i} + x_{n,m_i}) \left( 1 + \sum_{n=1}^{N} \sum_{m=1}^{M} c_{u,m}^{(n,i)} x_{u,m} \right)
- \frac{\hat{K} \alpha_n (\bar{x}_{n,m_1} + x_{n,m_1}) + (\bar{x}_{n,m_2} + x_{n,m_2})}{\gamma_n (\bar{x}_{n,m_1} + \bar{x}_{n,m_2})} \leq 0
\] (13)

which represents a quadratic condition. Neglecting the quadratic terms

\[
(x_{n,m_1} c_{u,m}^{(n,i)} x_{u,m}),
\]

this condition may be synthetically written:

\[
\sum_{n=1}^{N} \sum_{m=1}^{M} d_{u,m}^{(n)} x_{u,m} \leq 0 \quad (n = 1, 2, \ldots, N).
\] (14)

(d) **Constant fuel and beryllium volume condition**

The beryllium replaces equal fuel volume. This is translated into the condition:

\[
\sum_{m=1}^{M} \gamma_{n,m} x_{n,m} = 0 \quad (n = 1, 2, \ldots, N)
\] (15)

where \( \gamma_{n,m} \) is a coefficient which reduces \( x_{n,m} \) into volume fractions.

(e) **Fixed beryllium amount condition**

To fix the amount \( W \) of beryllium (labelled with index \( m_3 \)) to be distributed within the system is fixed, it must be:

\[
\sum_{n=1}^{N} (\bar{x}_{n,m_3} + x_{n,m_3}) = W
\] (16)

where \( \bar{x}_{n,m_3} \) represent the amount of beryllium oxide before the optimization.
Use of generalized perturbation methods for optimization of reactor design

The total number of conditions is $3N + 1$ represented by $2N + 1$ equations and $N$ inequalities. A check to see whether there are real solutions can be made by the drastic reduction to one subregion only. We see, as expected, that the equations are reduced to three, allowing only one solution (three being also the number of the interchangeable materials), if this is permitted by the inequalities.

In the procedure followed we introduced a few inaccuracies by linearizing the constraints (5) and (13). If more accurate solutions are required, a code should be developed adopting convex programming techniques, for instance the iterative method (GRIFFITH and STEWARD, 1961) or that of the penalty function (FIACCO and MCCORMICK, 1967).

In order to have information about the influence of this optimization on the reactor behaviour, other parametric calculations might be of interest once the values $x_{m,n}$ have been evaluated. One of these calculations may be relevant to the change of the sodium void reactivity effect $\rho_{Na}$. Other calculations might be relevant to changes of significant spectral indexes, such as the quantity:

$$R_s = \int_{R_{test}}^{R_{test}} \int_{0}^{1\text{keV}} \varphi(E) dE$$

The variations $\delta \rho_{Na}/\rho_{Na}$ and $\delta R_s/R_s$ may also be computed by using the generalized perturbation techniques mentioned above. If required, conditions imposed on the softness (or hardness) of the neutron spectrum might be easily considered as supplementary constraints to the optimization problem.

4. NUMERICAL EXAMPLE

A numerical example was performed relevant to the design of the material test reactor PEC (AIELLO et al., 1966) which is a sodium cooled fast system fuelled with enriched uranium oxide. The core is a cylinder with a height/diameter ratio close to one. The inner and the outer radii of the four subregions of the driver core are shown in Table 1. The calculations were made in infinite cylindrical geometry adopting the multigroup diffusion approximation and the cross section library by ABAGIAN et al. (1964). Use was made of the TAIM Code (DAL BONO, 1966) for the real and adjoint flux calculations, while the importance functions and the generalized perturbation calculations were performed by the CIAIP-1D and the GLOBPERT-1D Codes, respectively (DAL BONO et al., 1968). Finally, a linear programming code has been written using standard techniques.

The results of the calculations are presented in Tables 2 and 3. In Table 2 the optimum volume fraction distribution of the beryllium oxide in the four driver subregions is shown as a function of the average volume fraction of the beryllium oxide in the
core. To be noticed the tendency of the beryllium distribution to spread from inner subregions to outer ones with increasing average volume fraction of the beryllium. This fact is consequent, on one hand, from the limitation on the pin power and, on the other hand, from two main mechanisms which are in conflict with each other. These two mechanisms may be directly related to the numerator and denominator terms in the ratio at the right hand side of equation (1), which represents the Doppler effect. Once the total amount of beryllium is fixed, the first mechanism tends to push it toward the inner subregions, in order that the resonance neutron flux is enhanced where its importance is higher. On the contrary, the second mechanism tends to push the beryllium toward the outer subregions, where it has a major benefit on the neutron leakage and, therefore, on the critical mass reduction. This, in turn, makes the system more reactive and consequently enhances the reactivity associated to the Doppler effect. Besides, in the latter case, there is also a further contribution to the Doppler effect.

<table>
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<th>VF-BeO in the driver</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<td>0.05</td>
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<td>0</td>
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<td>0.061</td>
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<td>0.328</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2.—Volume fraction of BeO in driver core subregions after optimization for varying core average BeO volume fraction (VF-BeO)

<table>
<thead>
<tr>
<th>VF-BeO in driver</th>
<th>0.05*</th>
<th>0.05†</th>
<th>0.10†</th>
<th>0.15†</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.238</td>
<td>0.300</td>
<td>0.537</td>
<td>0.605</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.—Doppler effect increase and related characteristics after optimization for varying core average BeO volume fraction (VF-BeO)

* Uniform distribution.
† Optimized distribution.
\( \Delta K/K \) (Doppler coefficient in absence of BeO in the driver).
§ Critical mass in absence of beryllium: 372 Kg.
effect from the increase of the volume fraction of $^{238}\text{U}$, resulting from the constancy of the fuel plus beryllium volume fraction. In Table 3 the fractional increases of the Doppler effect are presented for the various cases considered, together with the resulting $^{235}\text{U}$ enrichment, the specific power fraction, the quantity of $^{235}\text{U}$ in the four core subregions, the integrated neutron flux below 1 keV with respect to the total flux, and finally, the power fraction of the test region.

As may be seen from the results, the Doppler effect increases are of the order of 50 per cent for most cases considered in the optimization. The most interesting case seems to be the one corresponding to an average fraction of the beryllium oxide in the core of 15 per cent, since to an increase of the Doppler effect of the order of 60 per cent corresponds a reduction of the critical mass of about 60 kg of $^{235}\text{U}$, without significant changes, if any, for what concerns the quality of the spectrum hardness and the power fraction of the test region. Besides, we observe, for this case, specific power fractions almost flat in the first three driver subregions with a 50 per cent reduction in the fourth one, which represents approximately 50 per cent of the overall fuel. This fact might induce one to optimize further the reactor design in order to adopt the simple fuel strategy which may be derived. In other words, once the maximum fuel burn-up is fixed, the outer elements could be extracted with a period twice as long as that corresponding to the inner ones.

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REFERENCES


