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APPLICATION OF THE METHOD OF STEEPEST DESCENT TO LAMINATED SHIELD WEIGHT OPTIMIZATION WITH SEVERAL CONSTRAINTS - THEORY

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16. Abstract

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APPLICATION OF THE METHOD OF STEEPEST DESCENT TO LAMINATED SHIELD WEIGHT OPTIMIZATION WITH SEVERAL CONSTRAINTS - THEORY

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SUMMARY

The method of steepest descent used in optimizing one-dimensional layered radiation shields has been extended to multidimensional, multiconstraint situations. The multidimensional optimization algorithm and equations have been developed for the case of a dose constraint in any one direction being dependent only on the shield thicknesses in that direction and independent of shield thicknesses in other directions. Expressions are derived for one-, two-, and three-dimensional cases (one, two, and three constraints). The procedure is applicable to the optimization of shields where there are different dose constraints and layering arrangements in the principal directions.

INTRODUCTION

One-dimensional shield weight optimization procedures are currently in use for the design of layered radiation shields (refs. 1 to 4). In general, though, shields such as for space power reactor applications may have different dose constraints in the several different directions. This requires either the superposition of two (or more) separate one-dimensional optimizations or development of a procedure which optimizes in two or more directions simultaneously. The basis for a computer code to do the latter is developed in this report. Expressions for the general case of constraints being functions of all shield layer thicknesses are derived, but the complete algorithm for the optimization procedure is made in this report only for the case where the dose constraint in each principal direction is a function of thicknesses in that direction only. This has application to the optimization of shields where there are different dose constraints and layering arrangements in the different principal directions and there is a weak (or no) dependence of the dose in one direction on the thickness in another direction.

The development of the method described in this report is parallel to the one-dimensional method developed by Bernick (ref. 3), programmed as the OPEX code (ref. 4), and later reprogrammed and reinterpreted as the OPEX-II code (ref. 5).

MATHEMATICAL STATEMENT OF THE PROBLEM

Assume a shield consisting of n layers. (For purposes of mathematical development, only the total number of layers need be considered. The n layers may be considered to be divided into n_1 layers in the first direction, n_2 layers in the second direction, and so forth, with $n = n_1 + n_2 + ...$) x_i is the thickness of the ith layer.

Let a vector $\overline{x}$ be defined in n-dimensional vector space with quantities x_1, x_2, . . ., x_n as components:

$$\overline{x} = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

Let the total shield weight be denoted by $W(\overline{x})$. The function $W(\overline{x})$ will in general be nonlinear.

The problem is then to minimize total shield weight subject to m dose constraints, say in certain directions. Mathematically, this can be expressed in the following way: Let

$$W(\overline{x}) \rightarrow \text{minimum} \tag{1}$$

with constraints

$$D_1^o = D_1(\overline{x}) - C_1 = 0 \tag{2a}$$

$$D_2^0 = D_2(\bar{x}) - C_2 = 0 \qquad (2b)$$

$$\vdots$$

$$D_m^0 = D_m(\bar{x}) - C_m = 0 \qquad (2m)$$

and

$$x_i \geq 0 \qquad (3)$$

where $D_j(\bar{x})$ is defined as the value of the dose rate at the j^{th} point (i. e., in the j^{th} direction) and is, in general, some nonlinear function of $\bar{x}$, and C_j is the required dose rate at point j. (Again, the x_i and hence D_j may be considered to be subdivided into the different directions with D_j strongly dependent on those x_i in the j^{th} direction and weakly dependent on, or completely independent of, the thicknesses in the other directions. The present derivation first considers the general case of D_j dependent on all x_i.)

Constraint (3) is necessary to ensure a solution with all $x_i \geq 0$, that is, a feasible solution.

THE ALGORITHM

The method of steepest descent as applied in this report is an iterative procedure to find a vector $\bar{x}_{min}$ which is a solution to the problem stated in equations (1), (2), and (3). The procedure is as follows:

(1) Choose an initial feasible vector $\bar{x}_0$, (i. e., one which satisfies constraints (2) and (3)).

(2) Find a unit vector $\bar{u}$, at point $\bar{x}_0$, which points in the direction of maximum allowable decrease in the function $W(\bar{x})$. The direction of $\bar{u}$ is chosen subject to the constraint that $\bar{u}$ is tangent to the constraint surface defined by $D_j^0(x) = 0$ for all j (i. e., the dose constraint is met).

(3) Calculate a vector $\bar{x}_1$

$$\bar{x}_1 = \bar{x}_0 + \lambda^0 \bar{u}$$

where λ^0 is some interation parameter, a constant, say.

(4) Calculate $D_j^o(\bar{x}_1)$ for all j. Because of the nonlinear nature of D, $D_j^o(\bar{x}_1)$ will not, in general, be equal to zero. A corrected point $\bar{x}_1$ is then determined such that

$$D_j^o(\bar{x}_1) = 0$$

(5) Set $\bar{x}_1 \rightarrow \bar{x}_0$; repeat steps (2) to (5) until some convergence criterion on weight is satisfied. The final value of $\bar{x}$ thus computed should then be a close approximation of $\bar{x}_{min}$.

DERIVATION OF $\bar{u}$

General Considerations

Let vectors $\bar{g}$, and $\bar{a}_1, \bar{a}_2, \ldots, \bar{a}_m$ be defined by

$$\bar{g} = \nabla W(\bar{x})$$

$$\bar{a}_1 = \nabla D_1^o(\bar{x})$$

$$\bar{a}_2 = \nabla D_2^o(\bar{x})$$

$$\vdots$$

$$\bar{a}_m = \nabla D_m^o(\bar{x})$$

where

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial}{\partial x_n} \end{bmatrix}$$

and ∇ is the conventional gradient operator as applied in n-dimensional space. The problem is then to find a vector $\bar{u}$ at some point $\bar{x}$ such that

$$\bar{g} \cdot \bar{u} \rightarrow \text{minimum} \tag{4}$$

$$\bar{u} \cdot \bar{u} = 1 \tag{5}$$

$$\bar{a}_1 \cdot \bar{u} = 0 \tag{6a}$$

$$\bar{a}_2 \cdot \bar{u} = 0 \tag{6b}$$

$$\begin{matrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{matrix}$$

$$\bar{a}_m \cdot \bar{u} = 0 \tag{6m}$$

Expression (4) indicates that the component of $\bar{u}$ along the direction of greatest increase of W is to be minimized (i. e., the component in the direction of greatest decrease of W is to be maximized). In the case of no dose constraints, for example, $\bar{u}$ and $\bar{g}$ would point in opposite directions or

$$\frac{\bar{g} \cdot \bar{u}}{\bar{g}} = -1$$

Expression (5) constrains $\bar{u}$ to be a unit vector. This is added for computational convenience. Expressions (6) simply state that $\bar{u}$ must be perpendicular to ∇D_j^o (i. e., $\bar{u}$ must lie in the plane of, or in general only be tangent to, a hypersurface of constant dose, $D_j^o = 0$, for all j).

Equations (4) to (6) can be solved by the method of Lagrange multipliers. Write the Lagrangian as

$$\mathscr{L} = \bar{g} \cdot \bar{u} + \alpha_1(\bar{a}_1 \cdot \bar{u}) + \alpha_2(\bar{a}_2 \cdot \bar{u}) + \ldots - \beta((\bar{u} \cdot \bar{u}) - 1) \tag{7}$$

where $\alpha_1, \alpha_2, \ldots \alpha_m$, and β are undetermined multipliers. The stationary points of the objective function $\bar{g} \cdot \bar{u}$ are desired at a particular point $\bar{x}$. At this particular point, $\bar{g}$ is fixed and only the components of $\bar{u}$ are variable; that is, $\bar{g} \cdot \bar{u} = \bar{g} \cdot \bar{u}(u_i)$ only. Therefore, to solve for the unknown u_i and multipliers α_i and β, each partial derivative of $\mathscr{L}$, equation (7), with respect to u_i is set equal to zero to determine stationary points. That is,

$$\frac{\partial \mathscr{L}}{\partial u_1} = 0$$

$$\frac{\partial \mathscr{L}}{\partial u_2} = 0$$

$$\vdots$$

$$\frac{\partial \mathscr{L}}{\partial u_n} = 0$$

or simply

$$\nabla_{\overline{u}} \mathscr{L} = 0$$

Evaluating this term by term, where $\hat{u}_i$ is a unit vector in the i^{th} direction,

$$\nabla_{\overline{u}}(\overline{g} \cdot \overline{u}) = \sum_{i=1}^{n} \hat{u}_i \frac{\partial}{\partial u_i} (g_1 \cdot u_1 + g_2 \cdot u_2 + \ldots + g_n \cdot u_n)$$

$$= \left[g_1 \left(\hat{u}_1 \frac{\partial u_1}{\partial u_1} \right) + g_2 \left(\hat{u}_2 \frac{\partial u_2}{\partial u_2} \right) + \ldots \; g_n \left(\hat{u}_n \frac{\partial u_n}{\partial u_n} \right) \right]$$

$$= \sum_{i=1}^{n} g_i \hat{u}_i = \overline{g}$$

Similarly,

$$\nabla_{\overline{u}}(\alpha_i \overline{a}_i \cdot \overline{u}) = \alpha_i \overline{a}_i$$

and

$$\nabla_{\bar{u}}(\bar{u} \cdot \bar{u}) = \sum_{i=1}^{n} \hat{u}_i \frac{\partial}{\partial u_i} (u_1 \cdot u_1 + u_2 \cdot u_2 + \ldots + u_n \cdot u_n)$$

$$= \sum_{i=1}^{n} \hat{u}_i \frac{\partial}{\partial u_i} \left(u_i^2\right) = \sum_{i=1}^{n} \hat{u}_i 2u_i = 2\bar{u}$$

or finally

$$\nabla_{\bar{u}} \mathscr{L} = 0 = \bar{g} + \alpha_1 \bar{a}_1 + \alpha_2 \bar{a}_2 + \ldots - 2\beta\bar{u} \tag{8}$$

Derivation of α_i

Equation (8) along with constraints (5) and (6a) to (6m) provide a set of $m + 2$ equations in $m + 2$ unknowns ($\bar{u}$, β, α_1, α_2, . . ., α_m). To solve this set of equations, take $a_1 \cdot$ [eq. (8)] and obtain

$$\bar{g} \cdot \bar{a}_1 + \alpha_1 a_1^2 + \alpha_2 \bar{a}_1 \cdot \bar{a}_2 + \ldots + \alpha_m \bar{a}_1 \cdot \bar{a}_m - 2\beta \bar{a}_1 \cdot \bar{u} = 0 \tag{9a}$$

Then take $\bar{a}_2 \cdot$ [eq. (8)] and obtain

$$\bar{g} \cdot \bar{a}_2 + \alpha_1 \bar{a}_2 \cdot \bar{a}_1 + \alpha_2 a_2^2 + \ldots + \alpha_m \bar{a}_2 \cdot \bar{a}_m - 2\beta \bar{a}_2 \cdot \bar{u} = 0 \tag{9b}$$

$$\vdots$$

$$\bar{g} \cdot \bar{a}_m + \alpha_1 \bar{a}_m \cdot \bar{a}_1 + \alpha_2 \bar{a}_m \cdot \bar{a}_2 + \ldots + \alpha_m \bar{a}_m \cdot \bar{a}_m - 2\beta \bar{a}_m \cdot \bar{u} = 0 \tag{9m}$$

Because of boundary condition (6), terms like $\bar{a}_i \cdot \bar{u}$ vanish. Hence, equations (9) compose a set of m equations in m unknowns, namely,

$$
\begin{bmatrix}
\bar{a}_1 \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_2 & \cdots & \bar{a}_1 \cdot \bar{a}_m \\
\bar{a}_2 \cdot \bar{a}_1 & \bar{a}_2 \cdot \bar{a}_2 & \cdots & \bar{a}_2 \cdot \bar{a}_m \\
 & & \vdots & \\
\bar{a}_m \cdot \bar{a}_1 & \bar{a}_m \cdot \bar{a}_2 & \cdots & \bar{a}_m \cdot \bar{a}_m
\end{bmatrix}
\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{bmatrix}
=
\begin{bmatrix} -\bar{g} \cdot \bar{a}_1 \\ -\bar{g} \cdot \bar{a}_2 \\ \vdots \\ -\bar{g} \cdot \bar{a}_m \end{bmatrix}
\tag{10}
$$

In principle, equation (10) can be solved for any m. Consider the following cases:
m = 1:

$$
\alpha_1 = \frac{-\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}
\tag{11}
$$

m = 2:

Let

$$
D_2 = \det\begin{pmatrix} \bar{a}_1 \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_2 \\ \bar{a}_2 \cdot \bar{a}_1 & \bar{a}_2 \cdot \bar{a}_2 \end{pmatrix} = (\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2) - (\bar{a}_2 \cdot \bar{a}_1)(\bar{a}_1 \cdot \bar{a}_2)
$$

Then

$$
\alpha_1 = \frac{\begin{pmatrix} -\bar{g} \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_2 \\ -g \cdot \bar{a}_2 & \bar{a}_2 \cdot \bar{a}_2 \end{pmatrix}}{D_2} = \frac{-(\bar{g} \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2) + (\bar{g} \cdot \bar{a}_2)(\bar{a}_1 \cdot \bar{a}_2)}{(\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2) - (\bar{a}_2 \cdot \bar{a}_1)^2}
\tag{12a}
$$

$$
\alpha_2 = \frac{\begin{pmatrix} \bar{a}_1 \cdot \bar{a}_1 & -\bar{g} \cdot \bar{a}_1 \\ \bar{a}_2 \cdot \bar{a}_1 & -\bar{g} \cdot \bar{a}_2 \end{pmatrix}}{D_2} = \frac{-(\bar{a}_1 \cdot \bar{a}_1)(\bar{g} \cdot \bar{a}_2) + (\bar{g} \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_1)}{(\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2) - (\bar{a}_2 \cdot \bar{a}_1)^2}
\tag{12b}
$$

m = 3:

Let

$$D_3 = \det\begin{pmatrix} \bar{a}_1 \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_2 & \bar{a}_1 \cdot \bar{a}_3 \\ \bar{a}_2 \cdot \bar{a}_1 & \bar{a}_2 \cdot \bar{a}_2 & \bar{a}_2 \cdot \bar{a}_3 \\ \bar{a}_3 \cdot \bar{a}_1 & \bar{a}_3 \cdot \bar{a}_2 & \bar{a}_3 \cdot \bar{a}_3 \end{pmatrix} = (\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2)(\bar{a}_3 \cdot \bar{a}_3)$$

$$-(\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_3)^2 - (\bar{a}_1 \cdot \bar{a}_2)^2(\bar{a}_3 \cdot \bar{a}_3)$$

$$+(\bar{a}_1 \cdot \bar{a}_2)(\bar{a}_2 \cdot \bar{a}_3)(\bar{a}_1 \cdot \bar{a}_3)$$

$$+(\bar{a}_1 \cdot \bar{a}_3)(\bar{a}_2 \cdot \bar{a}_1)(\bar{a}_3 \cdot \bar{a}_2)$$

$$-(\bar{a}_1 \cdot \bar{a}_3)^2(\bar{a}_2 \cdot \bar{a}_2)$$

Then

$$\alpha_1 = \frac{\begin{pmatrix} -\bar{g} \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_2 & \bar{a}_1 \cdot \bar{a}_3 \\ -\bar{g} \cdot \bar{a}_2 & \bar{a}_2 \cdot \bar{a}_2 & \bar{a}_2 \cdot \bar{a}_3 \\ -\bar{g} \cdot \bar{a}_3 & \bar{a}_3 \cdot \bar{a}_2 & \bar{a}_3 \cdot \bar{a}_3 \end{pmatrix}}{D_3} \tag{13a}$$

$$\alpha_2 = \frac{\begin{pmatrix} \bar{a}_1 \cdot \bar{a}_1 & -\bar{g} \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_3 \\ \bar{a}_2 \cdot \bar{a}_1 & -\bar{g} \cdot \bar{a}_2 & \bar{a}_2 \cdot \bar{a}_3 \\ \bar{a}_3 \cdot \bar{a}_1 & -\bar{g} \cdot \bar{a}_3 & \bar{a}_3 \cdot \bar{a}_3 \end{pmatrix}}{D_3} \tag{13b}$$

$$\alpha_3 = \frac{\begin{pmatrix} \bar{a}_1 \cdot \bar{a}_1 & \bar{a}_1 \cdot \bar{a}_2 & -\bar{g} \cdot \bar{a}_1 \\ \bar{a}_2 \cdot \bar{a}_1 & \bar{a}_2 \cdot \bar{a}_2 & -\bar{g} \cdot \bar{a}_2 \\ \bar{a}_3 \cdot \bar{a}_1 & \bar{a}_3 \cdot \bar{a}_2 & -\bar{g} \cdot \bar{a}_3 \end{pmatrix}}{D_3} \tag{13c}$$

Derivation of β and $\bar{u}$

To solve for β, rearrange equation (8):

$$u = \frac{\bar{g} + \alpha_1\bar{a}_1 + \alpha_2\bar{a}_2 + \cdot \cdot \cdot \alpha_m\bar{a}_m}{2\beta} \tag{14}$$

Take $\bar{u}\cdot$ of both sides. Using both equation (14) and $\bar{u} \cdot \bar{u} = 1$ results in

$$\bar{u} \cdot \bar{u} = 1 = \frac{(\bar{g} + \alpha_1\bar{a}_1 + \alpha_2\bar{a}_2 + \cdot \cdot \cdot + \alpha_m\bar{a}_m)}{2\beta} \cdot \frac{(\bar{g} + \alpha_1\bar{a}_1 + \alpha_2\bar{a}_2 + \cdot \cdot \cdot \alpha_m\bar{a}_m)}{2\beta} \tag{15}$$

<u>One constraint (m = 1).</u> - For $m = 1$, equation (15) reduces to

$$4\beta^2 = \bar{g} \cdot \bar{g} + 2\alpha_1\bar{a}_1 \cdot \bar{g} + \alpha_1^2(\bar{a}_1 \cdot \bar{a}_1)$$

From equation (11)

$$\alpha_1 = \frac{-\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}$$

So

$$4\beta^2 = \bar{g} \cdot \bar{g} - 2\left(\frac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}\right)(\bar{a}_1 \cdot \bar{g}) + \left(\frac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}\right)^2 (\bar{a}_1 \cdot \bar{a}_1) = \bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1}$$

$$2\beta = \pm\sqrt{\bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1}}$$

The sign of this has not yet been resolved.

From equation (14) and the value of α_1 from equation (11) we have for $m = 1$, then,

$$\bar{u} = \frac{\bar{g} - \left(\frac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}\right)\bar{a}_1}{\pm\left(\bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1}\right)^{1/2}} \tag{16}$$

For this to be a real solution, it is necessary that

$$\left[\bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1}\right] > 0 \tag{17}$$

Finally, the sign must be resolved.

Recall the original problem was to find the minimum $\bar{u} \cdot \bar{g}$. Therefore, taking $\bar{g} \cdot$ [eq. (16)] yields

$$\bar{u} \cdot \bar{g} = \frac{\bar{g} \cdot \bar{g} - \left(\frac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}\right)(\bar{a}_1 \cdot \bar{g})}{\pm\left(\bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1}\right)^{1/2}} \tag{18}$$

Or, with

$$B = \bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1}$$

Equation (18) becomes

$$\bar{u} \cdot \bar{g} = \frac{B}{\pm B^{1/2}}$$

Because it is necessary that $B > 0$ for a solution, the plus sign maximizes $\bar{u} \cdot \bar{g}$ and the minus sign minimizes $\bar{u} \cdot \bar{g}$. Therefore, the minus sign is the required solution for this problem.

Hence, the final solution for the $m = 1$ case is

$$\bar{u} = \frac{-\bar{g} + \left(\frac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}\right)\bar{a}_1}{\left[\bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{(\bar{a}_1 \cdot \bar{a}_1)}\right]^{1/2}} \tag{19}$$

This is the one-dimensional result derived by Bernick (ref. 3).

Two or three constraints ($m = 2$ or $m = 3$). - From equation (15), for $m = 2$,

$$4\beta^2 = (\bar{g} + \alpha_1\bar{a}_1 + \alpha_2\bar{a}_2) \cdot (\bar{g} + \alpha_1\bar{a}_1 + \alpha_2\bar{a}_2)$$

$$= \bar{g} \cdot \bar{g} + 2\alpha_1\bar{g} \cdot \bar{a}_1 + 2\alpha_2\bar{g} \cdot \bar{a}_2 + \alpha_1^2\bar{a}_1 \cdot \bar{a}_1 + 2\alpha_1\alpha_2\bar{a}_1 \cdot \bar{a}_2 + \alpha_2^2\bar{a}_2 \cdot \bar{a}_2 \tag{20}$$

This may be expanded by using the appropriate expressions for α, equation (12). From equation (14),

$$\bar{u} = \frac{\bar{g} + \alpha_1\bar{a}_1 + \alpha_2\bar{a}_2}{2\beta} \tag{21}$$

where α_1 and α_2 are obtained from equation (12) and β is obtained from equation (20). This is the general expression for the vector $\bar{u}$ for a two-constraint problem.

In general, the dose in any direction is known and may be expressed approximately as a function of thicknesses in that direction only. This report presently generates the optimization algorithm for this special case only. That is, consider the dose at points in the first and second (and third) directions determined only by the thicknesses in that particular direction. It is stated previously in this report that the n thicknesses generally might be regarded as being n_1 thicknesses in the first direction, n_2 in the second, and n_3 in the third and that $n_1 + n_2 + n_3 = n$. If the dose equations are

$$D_1^O = D_1^O(x_i) \qquad i = 1, n_1$$

$$D_2^O = D_2^O(x_i) \qquad i = (n_1 + 1), (n_1 + n_2)$$

$$D_3^O = D_3^O(x_i) \qquad i = (n_1 + n_2 + 1), n$$

one obtains

$$\bar{a}_1 = \begin{bmatrix} \frac{\partial D_1^o}{\partial x_1} \\ \frac{\partial D_1^o}{\partial x_2} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial D_1^o}{\partial x_{n_1}} \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \qquad \bar{a}_2 = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \frac{\partial D_2^o}{\partial x_{n_1+1}} \\ \frac{\partial D_2^o}{\partial x_{n_1+2}} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial D_2^o}{\partial x_{n_1+n_2}} \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \qquad \bar{a}_3 = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \frac{\partial D_3^o}{\partial x_{n_1+n_2+1}} \\ \frac{\partial D_3^o}{\partial x_{n_1+n_2+2}} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial D_3^o}{\partial x_n} \end{bmatrix}$$

As a result of this dose model, all terms of the form $\bar{a}_i \cdot \bar{a}_j$ equal 0 for $i \neq j$. Although the dose terms in the different directions are decoupled, the weight derivatives are not.

For the two-constraint, two-direction problem (m = 2), the values of α, equation (12), reduce to

$$\alpha_1 = \frac{-\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}$$

and

$$\alpha_2 = \frac{-\bar{g} \cdot \bar{a}_2}{\bar{a}_2 \cdot \bar{a}_2}$$

From equation (15)

$$4\beta^2 = \bar{g} \cdot \bar{g} + 2\alpha_1\bar{a}_1 \cdot \bar{g} + 2\alpha_2\bar{a}_2 \cdot \bar{g} + \alpha_1^2 a_1^2 + \alpha_2^2 a_2^2$$

$$= \bar{g} \cdot \bar{g} - 2\frac{(\bar{a}_1 \cdot \bar{g})^2}{\bar{a}_1 \cdot \bar{a}_1} - 2\frac{(\bar{a}_2 \cdot \bar{g})^2}{\bar{a}_2 \cdot \bar{a}_2} + \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1} + \frac{(\bar{g} \cdot \bar{a}_2)^2}{\bar{a}_2 \cdot \bar{a}_2}$$

$$= \bar{g} \cdot \bar{g} - \frac{(\bar{a}_1 \cdot \bar{g})^2}{\bar{a}_1 \cdot \bar{a}_1} - \frac{(\bar{a}_2 \cdot \bar{g})^2}{\bar{a}_2 \cdot \bar{a}_2}$$

$$2\beta = \pm\left[\bar{g} \cdot \bar{g} - \frac{(\bar{a}_1 \cdot \bar{g})^2}{\bar{a}_1 \cdot \bar{a}_1} - \frac{(\bar{a}_2 \cdot \bar{g})^2}{\bar{a}_2 \cdot \bar{a}_2}\right]^{1/2}$$

Finally, from equation (14) and the expressions for α_1, α_2, and β just given,

$$\bar{u} = \frac{\bar{g} - \dfrac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}\bar{a}_1 - \dfrac{\bar{g} \cdot \bar{a}_2}{\bar{a}_2 \cdot \bar{a}_2}\bar{a}_2}{\pm\left[\bar{g} \cdot \bar{g} - \dfrac{(\bar{a}_1 \cdot \bar{g})^2}{\bar{a}_1 \cdot \bar{a}_1} - \dfrac{(\bar{a}_2 \cdot \bar{g})^2}{\bar{a}_2 \cdot \bar{a}_2}\right]^{1/2}} \tag{22}$$

For the reasons given previously, the minus sign in the denominator is again selected.

Similarly, for $m = 3$, from equation (13),

$$D_3 = (\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2)(\bar{a}_3 \cdot \bar{a}_3)$$

$$\alpha_1 = \frac{(-\bar{g} \cdot \bar{a}_1)(\bar{a}_2 \cdot \bar{a}_2)(\bar{a}_3 \cdot \bar{a}_3)}{D_3} = \frac{-\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1}$$

$$\alpha_2 = \frac{(-\bar{g} \cdot \bar{a}_2)(\bar{a}_1 \cdot \bar{a}_1)(\bar{a}_3 \cdot \bar{a}_3)}{D_3} = \frac{-\bar{g} \cdot \bar{a}_2}{\bar{a}_2 \cdot \bar{a}_2}$$

$$\alpha_3 = \frac{(-\bar{g} \cdot \bar{a}_3)(\bar{a}_2 \cdot \bar{a}_2)(\bar{a}_1 \cdot \bar{a}_1)}{D_3} = \frac{-\bar{g} \cdot \bar{a}_3}{\bar{a}_3 \cdot \bar{a}_3}$$

From equation (15),

$$4\beta^2 = \bar{g} \cdot \bar{g} + \alpha_1^2(\bar{a}_1 \cdot \bar{a}_1) + \alpha_2^2(\bar{a}_2 \cdot \bar{a}_2) + \alpha_3^2(\bar{a}_3 \cdot \bar{a}_3) + 2\alpha_1(\bar{g} \cdot \bar{a}_1) + 2\alpha_2(\bar{g} \cdot \bar{a}_2) + 2\alpha_2(\bar{g} \cdot \bar{a}_3)$$

$$= \bar{g} \cdot \bar{g} + \frac{(\bar{g} \cdot \bar{a}_1)^2}{(\bar{a}_1 \cdot \bar{a}_1)} + \frac{(\bar{g} \cdot \bar{a}_2)^2}{(\bar{a}_2 \cdot \bar{a}_2)} + \frac{(\bar{g} \cdot \bar{a}_3)^2}{(\bar{a}_3 \cdot \bar{a}_3)} - \frac{2(\bar{g} \cdot \bar{a}_1)^2}{(\bar{a}_1 \cdot \bar{a}_1)} - \frac{2(\bar{g} \cdot \bar{a}_2)^2}{(\bar{a}_2 \cdot \bar{a}_2)} - \frac{2(\bar{g} \cdot \bar{a}_3)^2}{(\bar{a}_3 \cdot \bar{a}_3)}$$

$$= \bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{(\bar{a}_1 \cdot \bar{a}_1)} - \frac{(\bar{g} \cdot \bar{a}_2)^2}{(\bar{a}_2 \cdot \bar{a}_2)} - \frac{(\bar{g} \cdot \bar{a}_3)^2}{(\bar{a}_3 \cdot \bar{a}_3)}$$

From equation (14),

$$\bar{u} = \frac{\bar{g} - \frac{\bar{g} \cdot \bar{a}_1}{\bar{a}_1 \cdot \bar{a}_1} \bar{a}_1 - \frac{\bar{g} \cdot \bar{a}_2}{\bar{a}_2 \cdot \bar{a}_2} \bar{a}_2 - \frac{\bar{g} \cdot \bar{a}_3}{\bar{a}_3 \cdot \bar{a}_3} \bar{a}_3}{\pm \left[\bar{g} \cdot \bar{g} - \frac{(\bar{g} \cdot \bar{a}_1)^2}{\bar{a}_1 \cdot \bar{a}_1} - \frac{(\bar{g} \cdot \bar{a}_2)^2}{\bar{a}_2 \cdot \bar{a}_2} - \frac{(\bar{g} \cdot \bar{a}_3)^2}{\bar{a}_3 \cdot \bar{a}_3} \right]^{1/2}} \tag{23}$$

Again the minus sign in the denominator is selected.

By comparing equations (19), (22), and (23), one could extend the derivation of $\bar{u}$ to even higher dimensions ($m > 3$). This is, however, only of academic interest because one could probably not define a dose-thickness relation to fit the m-dimensional case.

COMPLETION OF THE OPTIMIZATION ALGORITHM

Let the vector $\bar{u}$, evaluated by equation (19), (22), or (23) at $\bar{x}_k$, where k indicates the k^{th} optimization step, be denoted by $\bar{u}_k$. After $\bar{u}_k$ and $\bar{x}_{k+1}$ are determined from

$$\bar{x}_{k+1} = \bar{x}_k + \lambda^k \bar{u}_k \tag{24}$$

a dose rate calculation is made. If the quantity $D_1^o(\bar{x}_{k+1})$ (see eq. (2)) is sufficiently different from zero, a correction to $\bar{x}_{k+1}$ must be made. An increment $d\bar{x}_{k+1}$ with components $dx_1, \ldots, dx_n$ is sought such that

$$D_i^o(\bar{x}_{k+1}) - \delta D(\bar{x}_{k+1}) = 0 \tag{25}$$

where

$$\delta D(\bar{x}_{k+1}) = \nabla D_i^o(\bar{x}_{k+1}) \cdot \overline{dx}_{k+1} \tag{26}$$

Also a minimum $|\overline{dx}_{k+1}|$ is desired.

This problem is then to minimize $\overline{dx} \cdot \overline{dx}$ with the constraint

$$\delta D(\bar{x}_{k+1}) = D_i^o(\bar{x}_{k+1})$$

Again define a Lagrangian $\mathscr{L}$ by

$$\mathscr{L} = \overline{dx} \cdot \overline{dx} + \gamma[\delta D(\bar{x}_{k+1}) - D_i^o(\bar{x}_{k+1})] \tag{27}$$

where γ is an undetermined multiplier. We wish to find stationary points of the objective function $\overline{dx} \cdot \overline{dx}$ at $\bar{x}_{k+1}$. To solve for the unknown dx_i and multiplier γ, at the stationary points, again take derivatives of $\mathscr{L}$, equation (27), with respect to dx_i and set each equal to zero. The result is

$$\left.\begin{aligned} \frac{\partial \mathscr{L}}{\partial dx_1} &= 0 = 2dx_1 + \gamma \nabla D_i^o(\bar{x}_{k+1}) \cdot \hat{dx}_1 \\ &\vdots \\ \frac{\partial \mathscr{L}}{\partial dx_n} &= 0 = 2dx_n + \gamma \nabla D_i^o(x_{k+1}) \cdot \hat{dx}_n \end{aligned}\right\} \tag{28}$$

where $\hat{dx}_i$ is a unit vector in the direction $\overline{dx}_i$. Equations (28) may be written as

$$0 = 2\overline{dx} + \gamma \nabla D_i^o(x_{k+1}) \tag{29}$$

Equations (25) and (29) provide a set of $n + 1$ equations in $n + 1$ unknowns dx_i and γ. To solve this, from equation (29), we have

$$\overline{dx} = \frac{-\gamma}{2} \nabla D_i^o(\bar{x}_{k+1})$$

Substituting this in equation (25) and using equation (26) give

$$D_i^o(\bar{x}_{k+1}) - \nabla D_i^o(\bar{x}_{k+1}) \cdot \left(\frac{-\gamma}{2}\right) \nabla D_i^o(\bar{x}_{k+1}) = 0$$

or

$$\gamma = \frac{-2D_i^o(\bar{x}_{k+1})}{\nabla^2 D_i^o(\bar{x}_{k+1})}$$

It follows, then, that

$$\overline{dx} = \frac{D_i^o(\overline{x}_{k+1}) \nabla D_i^o(\overline{x}_{k+1})}{\nabla^2 D_i^o(\overline{x}_{k+1})}$$

The new corrected vector $\overline{x}_{k+1}$ which satisfies the i^{th} dose constraint is given by

$$\overline{x}_{k+1} = \overline{x}_{k+1} + \overline{dx}$$

The procedure is to be repeated for each of the j directions.

The algorithm is terminated when the relative weight change from one iteration to the next is less than some prescribed ϵ. That is, when

$$\left| \frac{W(\overline{x}_{k+1}) - W(\overline{x}_k)}{W(\overline{x}_k)} \right| < \epsilon$$

CONCLUDING REMARKS

The algorithm for optimizing a two- or three-dimensional shield has been developed by extending a one-dimensional algorithm. Equations have been derived which permit implementation of this algorithm in a computer program similar to existing one-dimensional optimization codes.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, September 17, 1971,
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