APPLICATION OF PONTRYAGIN'S PRINCIPLE OF THE MAXIMUM FOR FINDING THE OPTIMUM CONCENTRATION DISTRIBUTION OF FUEL IN A FLAT DISPERSE FUEL ELEMENT

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Pontryagin's principle of the maximum is used for finding the optimum fuel distribution in terms of the minimum temperature drop from the center to the edge of a disperse fuel element. The result is illustrated on a specific example.

Since recently, various mathematical methods have been successfully used for optimizing the characteristics of nuclear power plants. Along with the development and use of classical methods [1, 2], much attention has also been paid to Pontryagin's principle of the maximum [3, 4]. For optimization by the most common numerical methods [5, 6], the apparatus of coupled equations and the function of material effectiveness [7-10] have also been found very useful. In this article the authors will apply Pontryagin's principle of the maximum [11] to solving the problem of optimum fuel distribution with the minimum temperature drop in a flat disperse fuel element, which is very important from the standpoint of lowering the peak temperature and reducing the thermal stresses. One can obtain an analogous solution for a cylindrical heat emitting element. Fuel elements of the disperse type, made of fuel (UO_2, for example) embedded in a matrix (stainless steel, molybdenum, tungsten, etc.) have better thermophysical and strength characteristics then fuel elements of pure fuel. The thermal conductivity λ of a fuel and matrix mixture is a function of the thermal conductivities of its components and of the volume concentration of fuel ε:

$$\lambda = f(\varepsilon, \lambda_G, \lambda_M). \tag{1}$$

In order to solve the stated problem, it is necessary to obtain a minimum temperature drop ΔT between the center plane of the plate ($z = 0$) and its cooled edges ($z = \pm L$) at a given mean fuel concentration:

$$\bar{\varepsilon} = \frac{1}{L} \int_0^L \varepsilon(z) \, dz = \int_0^1 \varepsilon(\rho) \, d\rho \tag{2}$$

($\rho \equiv z/L$ is a dimensionless coordinate), at a given plate thickness $2L$, and at a given thermal flux density at the cooled plate edge

$$q = \int_0^L q_v(z) \, dz. \tag{3}$$

The meaning of condition (3) is that the power of a fuel element remains constant for the solution of their problem. The released heat q_V and the fuel concentration ε are related as follows:

$$q_v = A\varepsilon, \tag{4}$$

where $A = A[\varepsilon(\rho), \rho]$ is a functional determined by the neutron-physical design of a fuel element.

According to expression (1), the thermal conductivity of the mixture is an explicit function of coordinate z through ε. The differential equation of heat conduction for a heat emitting plate with $\lambda = \lambda(\varepsilon(z))$ is

$$\frac{d^2T}{dz^2} + \frac{1}{\lambda(\varepsilon(z))} \cdot \frac{d\lambda(\varepsilon(z))}{dz} \cdot \frac{dT}{dz} + \frac{q_v(z)}{\lambda(\varepsilon(z))} = 0;$$

with the boundary conditions $T = T(L)$ at $z = L$ and $dT/dz = 0$ at $z = 0$. Its solution is

$$\frac{dT}{dz} = -\frac{1}{\lambda\,(\varepsilon\,(z))} \int_0^z q_v\,(z')\,dz',$$

which yields

$$T\,(z) = -\int_0^z \frac{dz'}{\lambda\,(\varepsilon\,(z'))} \int_0^z q_v\,(z'')\,dz'' + C_1.$$

At $z = L$ we have $T = T(L)$ and, therefore,

$$T\,(z) = T\,(L) + \int_z^L \frac{dz'}{\lambda\,(\varepsilon\,(z'))} \int_0^{z'} q_v\,(z'')\,dz''.$$

The temperature drop $\Delta T = T(0) - T(L)$ is

$$\Delta T = \int_0^L \frac{dz'}{\lambda\,(\varepsilon\,(z'))} \int_0^{z'} q_v\,(z'')\,dz''. \tag{5}$$

This is the functional which must be minimized.

The subsequent analysis will show that the solution to this problem can be obtained even for a more general form of functional (5). In that case an additional neutro-physical design of the fuel element becomes necessary. Here, for simplicity, we will assume that both λ and q_V are linear functions of the fuel concentration ε:

$$\lambda = \lambda_M - (\lambda_M - \lambda_G)\,\varepsilon\,(z), \tag{6}$$

$$q_v = A\varepsilon\,(z) \quad (A = \text{idem}). \tag{7}$$

Relation (6) [12] is often used in practice. Assumption (7) is valid only in the case of a reactor with a rigid neutron spectrum and a small blocking effect. It then follows from the conditions $\bar{\varepsilon} = \text{idem}$ and $L = \text{idem}$ that also $q = \text{idem}$. Inserting (6) and (7) into (5) and replacing z by the dimensionless coordinate $\rho = z/L$, we obtain

$$\Delta T = \frac{AL^2}{\lambda_M} \int_0^1 \frac{\lambda_M d\rho}{\lambda\,(\rho)} \int_0^\rho \varepsilon\,(\rho')\,d\rho'.$$

This formula can be conveniently rewritten as

$$\theta = \frac{\Delta T \lambda_M}{AL^2} = \int_0^1 \frac{\int_0^\rho \varepsilon\,(\rho')\,d\rho'}{(1 - B\varepsilon\,(\rho))}\,d\rho, \tag{8}$$

where $B = 1 - \lambda_F/\lambda_M$ and $\theta = \Delta T \cdot \lambda_M/AL^2$ denotes the dimensionless temperature drop. Thus, in accordance with the originally formulated problem, it is necessary to find the fuel distribution $\varepsilon(\rho)$ $(0 \leq \varepsilon(\rho) \leq 1)$ across the plate thickness which minimizes functional (8) at a given mean fuel concentration $\bar{\varepsilon}$. We note that $0 \leq \bar{\varepsilon} \leq 1$ (see (2)) and $0 \leq B < 1$ when $\lambda_F \leq \lambda_M$.

For solving the problem we use Pontryagin's principle of the maximum, as it is immediately evident that with $\lambda_F = \lambda_M$ the entire fuel material is best placed at the plate edges corresponding to the extreme values of the solution 0 and 1 within the defined range. Consequently, the problem cannot be solved by the classical method of variational calculus. In accordance with [11], we introduce the following symbols:

$$x^0\,(\rho) = \int_0^\rho \frac{\int_0^{\rho''} \varepsilon\,(\rho')\,d\rho'}{(1 - B\varepsilon\,(\rho''))}\,d\rho'', \quad x^1\,(\rho) = \int_0^\rho \varepsilon\,(\rho')\,d\rho', \quad \varepsilon\,(\rho) \equiv u\,(\rho)$$

and, instead of functional (8), we will consider the following system of differential equations

$$\frac{dx^0\,(\rho)}{d\rho} = \frac{x^1\,(\rho)}{1 - Bu\,(\rho)}, \quad \frac{dx^1\,(\rho)}{d\rho} = u\,(\rho) \tag{9}$$

with the boundary conditions $x^0(0) = 0$, $x^0(1) = \theta_{min}$, $x^1(0) = 0$, $x^1(1) = \bar{\varepsilon}$. Thus, the problem has been reduced to that of finding the optimum control $u(\rho)$ and the corresponding trajectory in the phase space

(x^0, x^1) which will yield the minimum coordinate $x^1(1)$ at point $\rho = 1$. In accordance with Pontryagin's principle of the maximum [11], we construct the auxiliary function

$$H = \Psi_0(\rho)\, \frac{x^1(\rho)}{1 - Bu(\rho)} + \Psi_1(\rho)\, u(\rho). \tag{10}$$

In order that the optimum process $(u(\rho),\ x^0(\rho),\ x^1(\rho))$ can be found, there must exist a solution to the system of equations for functions Ψ_0, Ψ_1

$$\frac{d\Psi_0(\rho)}{d\rho} = -\frac{\partial H}{\partial x^0}, \quad \frac{d\Psi_1(\rho)}{d\rho} = -\frac{\partial H}{\partial x^1}, \tag{11}$$

with which the condition of the maximum

$$\sup_{0 < v \leqslant 1} H(\Psi_0,\ \Psi_1,\ x^1,\ v) = H(\Psi_0,\ \Psi_1,\ x^1,\ u). \tag{12}$$

will be satisfied at any point ρ on the interval $[0, 1]$.

From the first equation in (11) we have $\Psi_0 = \text{const}$. According to [11], we assume that $\Psi_0 = -1$. Then the solution to the second equation in (11) will be

$$\Psi_1(\rho) = \int_0^\rho \frac{d\rho'}{1 - Bu(\rho')} + C. \tag{13}$$

From the condition $x^1(1) = \bar{\varepsilon}$ one can determine C, but not explicitly. It will be explained here how this condition is to be used for solving the problem. The form of function $\Psi_1(\rho)$ indicates that it is a continuous increasing function.

Let us now examine function H in (10). From the standpoint of solving the system (11), we note that the first term on the right-hand side of (10) on the interval $[0, 1]$ represents a decreasing hyperbolic function of the variable u. The second term represents a straight line which, depending on the sign of function $\Psi_1(\rho)$, rises or falls within the interval $0 \leq u \leq 1$. It follows from there that function H of the variable u has either one maximum within the interval $[0, 1]$ or reaches its highest value at boundary $u = 0$ or boundary $u = 1$.

Before attempting to determine the optimum control, the equation for the derivative

$$\frac{\partial H}{\partial u} = -\frac{Bx^1(\rho)}{\left(1 - Bu(\rho)\right)^2} + \Psi_1(\rho) \tag{14}$$

will be used for revealing certain general properties of the optimum control.

Let us consider point $\rho = 0$. At this point $\partial H/\partial u = C$, i.e., the derivative has always the same sign and does not depend on u. Consequently, according to the principle of the maximum (12), $u(0) = 0$ when $C < 0$ or $u(0) = 1$ when $C > 0$. This is so because, with $C < 0$, function H only decreases and, therefore, reaches its maximum at $u = 0$, while with $C > 0$ it only increases and reaches its maximum at point $u = 1$.

When $C < 0$, there is an interval $0 \leq \rho \leq \rho_0$ where function $\Psi_1(\rho) < 0$ and thus $u(\rho) = 0$, inasmuch as $\partial H/\partial u < 0$ on this interval; furthermore, function $\Psi_1(\rho) = C + \rho$ (see (13)). The value of point

$$\rho_0 = -C \tag{15}$$

is obtained from the condition $\psi_1(\rho_0) = 0$. It follows from here that the fuel can only be placed above the point ρ_0.

We will now examine the value of u at point ρ_0. Since $x^1(\rho_0) = 0$ and $\psi_1(\rho_0) = 0$, hence series expansions of these functions in the vicinity of point ρ_0 on the right-hand side will together with (13) yield

$$x^1(\rho) = x^1(\rho_0) + \frac{dx^1(\rho_0)}{d\rho}(\rho - \rho_0) + \ldots + = u(\rho_0) \cdot (\rho - \rho_0),$$

$$\Psi_1(\rho) = \Psi_1(\rho_0) + \frac{d\Psi_1(\rho_0)}{d\rho}(\rho - \rho_0) + \ldots + = \frac{(\rho - \rho_0)}{1 - Bu(\rho_0)}.$$

Inserting these relations into (14), we obtain

$$\frac{\partial H}{\partial u}(\rho) = \frac{(\rho - \rho_0)}{1 - Bu(\rho_0)} \left(1 - \frac{Bu(\rho_0)}{1 - Bu(\rho_0)}\right). \tag{16}$$

If we assume that, when $\partial H/\partial u(\rho_0) = 0$, $u(\rho_0)$ assumes the value of some point within the interval $[0, 1]$ where it is defined, then Eq. (16) yields $u(\rho_0) = 1/2B$. For a realization of this case, parameter B must

have a value within the interval $0.5 \leq B \leq 1$, because $u(\rho_0)$ cannot exceed unity. An analysis of the expression inside the parentheses in Eq. (16), which completely determines the sign of the derivative, will also establish that $\partial H / \partial u(\rho) > 0$ near ρ_0 on the right-hand side, for any value of $u(\rho_0)$ with $0 \leq B < 0.5$. According to the principle of the maximum, this yields $u(\rho_0) = 1$. Consequently,

$$u(\rho_0) = \begin{cases} 1 & \text{for } 0 \leqslant B < 0.5, \\ \dfrac{1}{2B} & \text{for } 0.5 \leqslant B < 1. \end{cases} \tag{17}$$

It thus has been established that at point ρ_0 the value of function $u(\rho)$ jumps by ≥ 0.5.

We now proceed to the case where $C > 0$. It has been established earlier that here $u(0) = 1$. Function $u(\rho)$ must maintain this value also in the immediate vicinity of point $\rho = 0$. This follows from the form of the derivative (14) and expression (13). Let ρ_1 denote a point where $u(\rho) \neq 1$. An analysis of expression (14) with $u(\rho)$ assumed discontinuous at point ρ_1 will prove that, conversely, function $u(\rho)$ is continuous at this point. Therefore, the condition $\partial H / \partial u(\rho_1) = 0$ will yield an expression for point ρ_1:

$$\rho_1 = C \frac{(1-B)^2}{(2B-1)} . \tag{18}$$

Since always $\rho_1 \geq 0$, hence $C > 0$ only when $0.5 < B < 1$.

Thus, the preceding discussion has clarified some structural features of the optimum fuel distribution across the plate thickness. A complete solution to this problem will be sought by the method of successive approximations, applied to the following system of equations:

$$x^1(\rho) = \int_0^\rho u(\rho') \, d\rho', \tag{19}$$

$$\Psi_1(\rho) = \int_0^\rho \frac{d\rho'}{1 - Bu(\rho')} + C, \tag{20}$$

$$u(\rho) = \frac{1}{B} \left(1 - \sqrt{\frac{Bx^1(\rho)}{\Psi_1(\rho)}} \right) . \tag{21}$$

Expression (21) is obtained from (14) under the condition that $\partial H / \partial u = 0$, i.e., it describes the optimum fuel distribution for those values of ρ for which this distribution assumes values within the range where it is defined.

The general form of system (19)–(21) leads to the important conclusion that, when $C < 0$, the solution to the system is a constant not equal to zero on the interval $[\rho_0, 1]$. Indeed, denoting this solution by $\bar{u}$, we have

$$x^1(\rho) = \bar{u}(\rho - \rho_0) \text{ and } \Psi_0(\rho) = \frac{(\rho - \rho_0)}{1 + B\bar{u}} .$$

Inserting this function into expression (21), we find that $\bar{u} = 1/2B$ and this agrees exactly with the value of $u(\rho_0)$ (see (17)).

Taking into account expressions (16) and (17) for analyzing the sign of the derivative (14), we may conclude that for $0 \leq B < 0.5$ the function $u(\rho) = 1$ on the interval $[\rho_0, 1]$ when $C < 0$.

Thus, for negative values of the constant C we have obtained an analytical solution to the problem. For values of B within the interval $[0, 0.5]$

$$u_*(\rho) = \begin{cases} 0 & \text{for } 0 \leqslant \rho < \rho_0, \\ 1 & \text{for } \rho_0 \leqslant \rho \leqslant 1. \end{cases} \tag{22}$$

Moreover, $\rho_0 = 1 - \bar{\varepsilon}$, which follows from the condition that $x^1(1) = \bar{\varepsilon}$. For values of B within the upper interval $[0.5, 1]$ we have

$$u(\rho) = \begin{cases} 0 & \text{for } 0 \leqslant \rho < \rho_0, \\ \dfrac{1}{2B} & \text{for } \rho_0 \leqslant \rho \leqslant 1. \end{cases} \tag{23}$$

Here the boundary value of ρ_0 is determined from another expression $\rho_0 = 1 - 2\bar{\varepsilon}B$.

The solution to system (19)–(21) for positive values of the constant C is not as simple to formulate as for negative values. In this case calculations were made by the method of successive approximations.
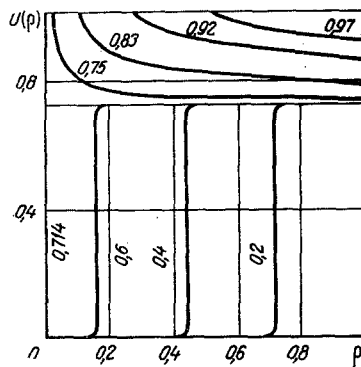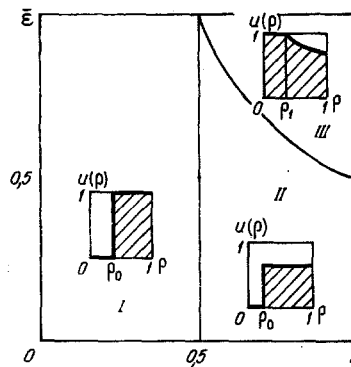
Fig. 1. Optimum fuel distribution across the thickness of a
flat fuel element, for various values of the mean volume con-
centration of fuel $\bar{\varepsilon}$ when B = 0.7.

Fig. 2. Trends of optimum fuel distributions across the plate
thickness, for various ranges of $\bar{\varepsilon}$ and B values.

Considering that the total quantity of fuel $\bar{\varepsilon}$ is uniquely related to the constant C, the value of the latter
was used as the initial parameter within the interval $[0, \ 2B-1/(1-B)^2]$ (see (18)). The calculation pro-
cedure by this method was as follows. With function $u(\rho) = 1$ on the interval $[0, \ \rho_1]$ and function $u(\rho_1)$ con-
tinuous at point ρ_1, we selected some zeroth approximation $u_0(\rho)$. Then, with the aid of expressions (19)
and (20), we calculated functions $x^1(\rho)$ and $\Psi_1(\rho)$.

Inserting these functions into (21) yielded the next (first) approximation $u_1(\rho)$, with which the calcula-
tion cycle was repeated, etc. The process was terminated when the maximum difference $|u_{n+1}(\rho)-u_n(\rho)|$
fell below some given value. Finally, with the aid of this solution, we determined the total quantity of fuel
$\bar{\varepsilon}$ corresponding to the originally assumed value of C. The iteration converged rather fast. For a solution
with an error not greater than 3%, it was necessary to go through 3-4 iteration cycles for the most rough
estimate of $u_0(\rho)$.

For illustration, the optimum fuel distribution across the plate thickness is shown in Fig. 1 for B
= 0.7 and various values of $\bar{\varepsilon}$. It is evident here that, as $\bar{\varepsilon}$ increases, the fuel fills in first from the plate
edges toward the center at a uniform concentration equal to 1/2B until $\bar{\varepsilon} = 1/2B$ ($\rho_0 = 0$). Then, as $\bar{\varepsilon}$ be-
gins to exceed this value slightly, there occurs a jump: $u(0) = 1$ along the interval $[0, \ \rho_1]$ where $u(\rho) = 1$,
and at $\rho > \rho_1$ the fuel concentration drops continuously toward the plate edge. As $\bar{\varepsilon}$ increases further, the
fuel fills in from the center toward the edge.

Thus, three characteristic modes of the solution to the problem have been established: (22), (23),
and the case where C > 0. Since any solution is uniquely determined by two parameters $\bar{\varepsilon}$ and B, hence in
the ($\bar{\varepsilon}$, B) space within the square $0 \le \bar{\varepsilon} \le 1$, $0 \le B \le 1$ to each mode corresponds a completely defined
region. These regions are shown in Fig. 2 along with the qualitative trend of the optimum fuel distribution
$u(\rho)$ for each. The boundary between regions II and III is established from the condition that $\rho_0 = 1-2\bar{\varepsilon}B$
= 0.

The large difference between the optimum distributions can be explained as follows. At small values
of B, when the thermal conductivities of both mixture components are close ($\lambda_F \simeq \lambda_M$), the fuel is best
placed at the plate edge (region I) from where heat can be removed more effectively. As the value of B in-
creases, with λ_F becoming smaller than λ_M, the placement of fuel at the edge begins to impede the heat
removal from inner layers and, therefore, the fuel must be diluted in the matrix material (region II). As
B increases still further and $\bar{\varepsilon}$ too, the fuel begins to block the heat flow from the plate to such an extent
that most of it must be placed at the center (region III).

We note that the optimum fuel distribution in regions I and II is very convenient from the standpoint
of technological design, because the fuel element is then made up of two zones with a uniform composition
each: the inner zone, moreover, containing only pure matrix material. This suggests that, when the values
of parameters B and $\bar{\varepsilon}$ lie within the ranges I and II, one should consider redesigning the fuel element
structure: the matrix material in the central zone does not serve as dilutant now for improving the ther-
mal conductivity of the mixture and, therefore, may be eliminated.

In conclusion, we consider the following comment to be in order. The preceding analysis of the problem applies to the case where the optimizing functional appears as a quadrature of a differential equation. In a more general case (multidimensionality, transiency, temperature-dependence of physical properties, etc.) the temperature of a fuel element can be determined only numerically. Linear temperature functionals can be minimized then with the mathematical apparatus of coupled equations of heat conduction [13] by the method shown in [6], for example.

NOTATION

λ_F, λ_M, λ	are the thermal conductivity of fuel, of matrix material, and of the mixture;
ε, $\bar{\varepsilon}$	are the volume concentration and mean volume concentration of fuel;
z	is the space coordinate;
L	is the half-thickness of fuel plate;
$\rho = z/L$	is the dimensionless coordinate;
q	is the thermal flux density at plate edge;
q_V	is the specific (per volume) heat generation;
$A = q_V/\varepsilon$	is the coefficient relating q_V and ε;
T	is the temperature;
ΔT	is the temperature drop between center and edge of plate;
$\theta = \Delta T \lambda_M / AL^2$	is the dimensionless temperature drop;
$B = 1 - \lambda_F/\lambda_M$	is the dimensionless parameter;
$u(\rho) \equiv \varepsilon(\rho)$	is the control function.

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