OPTIMIZATION OF A SYSTEM WITH DISTRIBUTED PARAMETERS

(OB ODNOI ZADACHE OPTIMIZATSII SISTEMY S RASPREDELENNYMI PARAMETRAMI)

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We shall consider the problem of the optimization of a succession of reactors.

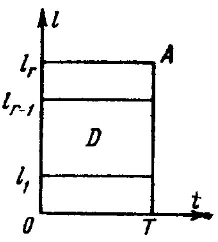
Let each reactor be described by the system of equations (see [1])

$$\frac{\partial x_i}{\partial l} = f_i(x, y) \qquad (i = 1, \ldots, n), \qquad \frac{\partial y_j}{\partial t} = \varphi_j(x, y) \qquad (j = 1, \ldots, p) \tag{1}$$

Here $x = (x_1, \ldots, x_n)$ is the vector variable which characterizes the state of the system in a given section of the reactor (concentration of substances, temperature, pressure and so on), $y = (y_1, \ldots, y_p)$ is the vector variable characterizing the state of the catalyzer, l is the running length of the reactor and t is the astronomic time.

Let us assume that the output of one of the components, x_1 for instance, must be optimized over the cycle time T. The controlling variables consist of some of the variables x_i (for instance, x_i for $i = n_1, \ldots, n$) on the input of each of the reactors. It can be easily seen that this problem can be expressed mathematically in the following manner.

Let us consider in the l, t plane the rectangle O, L, A, T. (We shall call it the region D). (Fig. 1.). Let us divide the segment $[O, L]$ into r parts defined by the points $l_1, \ldots, l_{r-1}$ We shall, respectively, denote by l_0 and l_r the end points of this segment. The points l_0 and l_r correspond to the beginnings and the ends of the reactors. Inside each rectangle



$$D_\alpha \ (l_\alpha \leqslant l \leqslant l_{\alpha+1}, \quad 0 \leqslant t \leqslant T; \ \alpha=0, \ldots, r-1)$$

the variables $x_i\ (l, t)$ satisfy the system (1).

On the lines $l = l_\alpha$, the variables $x_i\ (l, t)$ $(i = 1, \ldots, n_1 - 1)$ are continuous

$$x_i(l_\alpha - 0, t) = x_i(l_\alpha + 0, t)$$
$$(\alpha = 1, \ldots, r-1; \ i = 1, \ldots, n_1 - 1) \tag{2}$$

and the variables $x_i\ (l, t)\ (i = n_1, \ldots, n)$ can have discontinuities.

The functions $x_i\ (l_\alpha + 0, t)$ $(\alpha=0, \ldots, r-1; \ i=n_1, \ldots, n)$ have the physical meaning of distributed controlling parameters. It is assumed that these functions are piecewise continuous and piecewise continuously differentiable with respect to t. For $l = l_0$ and $t = t_0$ the following relations hold

$$x_i(l_0, t) = x_{i0}(t) \qquad (i = 1, \ldots, n_1 - 1) \tag{3}$$

$$y_j(l, 0) = y_{j0}(l) \qquad (j = 1, \ldots, p) \tag{4}$$

We shall assume that the functions $x_{i0}(t)$, $y_{j0}(l)$ are continuously differentiable. From the assumptions made, it follows that inside each rectangle D_α the variables $x_i(l, t)$ can have discontinuities only on the lines $t =$ constant, and that the $y_j(l, t)$ are continuous.

The optimum problem can now be formulated as follows. Find functions $x_i(l_\alpha + 0, t)$ $(\alpha = 0, \ldots, r - 1;\ i = n_1, \ldots, n)$, such that the integral

$$I = \int_0^T x_1(l_r, t)\, dt \tag{5}$$

takes a maximum value. We note that a number of papers [2–4] have appeared on the optimization of systems with distributed parameters. Here, we shall get the necessary conditions for having an extremum of the functional (5) and we shall consider one of the approximate methods for finding the optimum values of the controlling variables.

In place of the integral (5) let us consider the functional

$$I^* = \int_0^T x_1(l_r, t)\, dt + \sum_{\alpha=0}^{r-1} \int_{l_\alpha}^{l_{\alpha+1}} \int_0^T \Big[\sum_{i=1}^n \lambda_i (x_{il} - f_i(x, y)) + \sum_{j=1}^p \mu_j (y_{jt} - \varphi_j(x, y))\Big] dl\, dt$$
$$\left(x_{il} = \frac{\partial x_i}{\partial l},\quad y_{jt} = \frac{\partial y_j}{\partial t}\right) \tag{6}$$

Here the $\lambda_i = \lambda_i(l, t)$ are, thus far, completely arbitrary functions and the $\mu_j = \mu_j(l, t)$ are only constrained to be continuous in t.

If, in each rectangle D_α $(\alpha = 0, \ldots, r - 1)$ the functions x_i, y_j satisfy the system (1), the integral (6) will be equal to the integral (5) for any $x_i(l_\alpha + 0, t)$ $(\alpha = 0, \ldots, r - 1;\ i = n_1, \ldots, n)$.

Let us assume that for

$$x_i(l_\alpha + 0, t) = x_i^*(l_\alpha + 0, t) \qquad (\alpha = 0, \ldots, r - 1;\quad i = n_1, \ldots, n)$$

the functional I^* takes a maximum value. Let us vary $x_i^*(l_\alpha + 0, t)$.

We have

$$X_i(l_\alpha + 0, t) = x_i^*(l_\alpha + 0, t) + \delta x_i(l_\alpha + 0, t) \tag{7}$$

In order to find the variation of the functional (6) we shall first find the variation of the following functional

$$I_\alpha = \int_{l_\alpha}^{l_{\alpha+1}} \int_0^T F(z_1, \ldots, z_m, z_{1l}, \ldots, z_{ml}, z_{1t}, \ldots, z_{mt})\, dl\, dt \tag{8}$$

Here (9)

$$F = \sum_{i=1}^n \lambda_i (x_{il} - f_i) + \sum_{j=1}^p \mu_j (y_{jt} - \varphi_j), \qquad z_i = \begin{cases} x_i, & i = 1, \ldots, n \\ y_{i-n}, & i = n+1, \ldots, n+p = m \end{cases}$$

Let $z_i^*(l, t)$ correspond to the extremum functions $x_i^*(l_\alpha + 0, t)$.

The variation of the controlling variables (7) will yield a variation of the functions $z_i^*(l, t)$

$$Z_i(l, t) = z_i^*(l, t) + \eta_i(l, t) \tag{10}$$

We shall assume that inside each rectangle D_α the variables $\eta_i(l, t)$ are continuous and have continuous derivatives, whereupon the conditions

$$|\eta_i| < \varepsilon, \quad |\eta_{il}| < \varepsilon, \quad |\eta_{it}| < \varepsilon \tag{11}$$

are satisfied.

We shall find the variation of the functional (8) for $z_i(l, t) = z_i^*(l, t)$

$$\delta I_\alpha = \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} (F(z_i^* + \eta_i, z_{il}^* + \eta_{il}, z_{it}^* + \eta_{it}, l, t) - F(z_i^*, z_{il}^*, z_{it}^*, l, t))\, dl\, dt$$

Expanding the first integrand in a Taylor series and leaving only the small terms of the first order of magnitude, we get

$$\delta I_\alpha = \delta I' + \delta I'' + \delta I''', \qquad \delta I' = \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \frac{\partial F}{\partial z_i} \eta_i\, dl\, dt$$

$$\delta I'' = \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \frac{\partial F}{\partial z_{il}} \eta_{il}\, dl\, dt, \qquad \delta I''' = \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^{m'} \frac{\partial F}{\partial z_{it}} \eta_{it}\, dl\, dt \tag{12}$$

Integrating by parts and taking into account the continuity of $\mu_j(l, t) = \partial F / \partial z_{n+j,\, t}$ with respect to t, we get

$$\delta I'' = \int_0^T \sum_{i=1}^m \left(\frac{\partial F}{\partial z_{il}} \Big|_{l=l_{\alpha+1}-0} \eta_i(l_{\alpha+1} - 0, t) - \frac{\partial F}{\partial z_{il}} \Big|_{l=l_\alpha+0} \eta_i(l_\alpha + 0, t)\, dt - \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \frac{\partial}{\partial l} \left(\frac{\partial F}{\partial z_{il}} \right) \eta_i\, dl\, dt \tag{13}$$

$$\delta I''' = \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \left(\frac{\partial F}{\partial z_{it}} \Big|_{t=T} \eta_i(l, T) - \frac{\partial F}{\partial z_{it}} \Big|_{t=0} \eta_i(l, 0) \right) dl - \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \frac{\partial}{\partial t} \left(\frac{\partial F}{\partial z_{it}} \right) \eta_i\, dl\, dt \tag{14}$$

Substituting (13) and (14) into (12) we get

$$\delta I_\alpha = \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \left(\frac{\partial F}{\partial z_i} - \frac{\partial}{\partial l} \left(\frac{\partial F}{\partial z_{il}} \right) - \frac{\partial}{\partial t} \left(\frac{\partial F}{\partial z_{it}} \right) \right) \eta_i\, dl\, dt +$$

$$+ \int_0^T \sum_{i=1}^m \left(\frac{\partial F}{\partial z_{il}} \Big|_{l=l_{\alpha+1}-0} \eta_i(l_{\alpha+1} - 0, t) - \frac{\partial F}{\partial z_{il}} \Big|_{l=l_\alpha+0} \eta_i(l_\alpha + 0, t)\, dt + \right. \tag{15}$$

$$+ \int_{l_\alpha}^{l_{\alpha+1}} \sum_{i=1}^m \left(\frac{\partial F}{\partial z_{it}} \Big|_{t=T} \eta_i(l, T) - \frac{\partial F}{\partial z_{it}} \Big|_{t=0} \eta_i(l, 0) \right) dl$$

Using (9) this yields

$$\delta I_\alpha = \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \Big[\sum_{s=1}^{n} \Big(-\frac{\partial \lambda_s}{\partial l} - \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_s} \lambda_i - \sum_{j=1}^{p} \frac{\partial \varphi_j}{\partial x_s} \mu_j \Big) \delta x_s (l, t) + \tag{16}$$

$$+ \sum_{q=1}^{p} \Big(-\frac{\partial \mu_q}{\partial t} - \sum_{i=1}^{n} \frac{\partial f_i}{\partial y_q} \lambda_i - \sum_{j=1}^{p} \frac{\partial \varphi_j}{\partial y_q} \mu_j \Big) \delta y_q (l, t) \Big] dl\, dt +$$

$$+ \int_0^T \sum_{i=0}^{n} [\lambda_i (l_{\alpha+1} - 0, t)\, \delta x_i (l_{\alpha+1} - 0, t) - \lambda_i (l_\alpha + 0, t)\, \delta x_i (l_\alpha + 0, t)]\, dt +$$

$$+ \int_{l_\alpha}^{l_{\alpha+1}} \sum_{j=1}^{p} [\mu_j (l, T)\, \delta y_j (l, T) - \mu_j (l, 0)\, \delta y_j (l, 0)]\, dl$$

It follows that

$$\delta I^* = \int_0^T \delta x_1 (l_r, t)\, dt + \sum_{\alpha=0}^{r-1} \int_0^T \int_{l_\alpha}^{l_{\alpha+1}} \Big[\sum_{s=1}^{n} \Big(-\frac{\partial \lambda_s}{\partial l} - \sum_{i=1}^{n} \frac{\partial f_i}{\partial x_s} \lambda_i - \sum_{j=1}^{p} \frac{\partial \varphi_j}{\partial x_s} \mu_j \Big) \times$$

$$\times \delta x_s (l, t) + \sum_{q=1}^{p} \Big(-\frac{\partial \mu_q}{\partial t} - \sum_{i=1}^{n} \frac{\partial f_i}{\partial y_q} \lambda_i - \sum_{j=1}^{p} \frac{\partial \varphi_j}{\partial y_q} \mu_j \Big) \times \tag{17}$$

$$\times \delta y_q (l, t)]\, dl\, dt + \sum_{\alpha=0}^{r-1} \int_0^T \sum_{i=1}^{n} [\lambda_i (l_{\alpha+1} - 0, t) \times$$

$$\times \delta x_i (l_{\alpha+1} - 0, t) - \lambda_i (l_\alpha + 0, t)\, \delta x_i (l_\alpha + 0, t)]\, dt +$$

$$+ \int_{l_0}^{l_r} \sum_{j=1}^{p} [\mu_j (l, T)\, \delta y_j (l, T) - \mu_j (l, 0)\, \delta y_j (l, 0)]\, dl$$

We shall now choose functions λ_s $(s = 1, \ldots, n)$, μ_q $(q = 1, \ldots, p)$ which satisfy the system of equations

$$\frac{\partial \lambda_s}{\partial l} = -\sum_{i=1}^{n} \frac{\partial f_i}{\partial x_s} \lambda_i - \sum_{j=1}^{p} \frac{\partial \varphi_j}{\partial x_s} \mu_j \qquad (s = 1, \ldots, n)$$

$$\frac{\partial \mu_q}{\partial t} = -\sum_{i=1}^{n} \frac{\partial f_i}{\partial y_q} \lambda_i - \sum_{j=1}^{p} \frac{\partial \varphi_j}{\partial y_q} \mu_j \qquad (q = 1, \ldots, p) \tag{18}$$

We shall, furthermore, assume that on the lines

$$l = l_\alpha \quad (\alpha = 1, \ldots, r - 1), \qquad \lambda_s (l_\alpha - 0, t) = \lambda_s (l_\alpha + 0, t) = \lambda_s (l_\alpha, t) \quad (s = 1, \ldots, n) \tag{19}$$

and that, at the boundary of the region D for $l = l_\alpha$ and $t = T$, the equations

$$\lambda_1 (l_r, t) = 1, \qquad \lambda_s (l_r, t) = 0 \quad (s = 2, \ldots, n), \qquad \mu_q (l, T) = 0 \quad (q = 1, \ldots, p) \tag{20}$$

are satisfied.

For such a choice of λ_s and μ_q the double integral in (17) becomes equal to zero. Noticing also that on the basis of (2) – (4)

$$\delta x_i\,(l_\alpha - 0,\,t) = \delta x_i\,(l_\alpha + 0,\,t) \qquad (\alpha = 1,\ldots, r-1;\; i = 1,\ldots, n_1 - 1) \quad (21)$$

$$\delta x_i\,(l_0,\,t) = \delta y_j\,(l,\,0) = 0 \qquad (i = 1,\ldots, n_1 - 1;\; j = 1,\ldots, p) \quad (22)$$

we get the following expression for the variations of the functional I

$$\delta I = \delta I^* = -\sum_{\alpha=1}^{r-1}\int_0^T \sum_{i=n_1}^{n} (\delta x_i\,(l_\alpha + 0,\,t) - \delta x_i\,(l_\alpha - 0,\,t))\,\lambda_i\,(l_\alpha,\,t)\,dt - -\int_0^T \sum_{i=n_1}^{n} \delta x_i\,(l_0,\,t)\,\lambda_i\,(l_0,\,t)\,dt \quad (23)$$

It can be easily shown [5], that $\delta I = 0$ on the extremes of the functional I. Whereupon, by virtue of the independence of the variations $\delta x_i\,(l_\alpha + 0,\,t)$ $(\alpha = 0,\ldots, r-1;\; i = n_1,\ldots, n)$ we have

$$\lambda_i\,(l_\alpha,\,t) = 0 \qquad (\alpha = 0,\ldots, r-1;\; i = n_1,\ldots, n) \quad (24)$$

Thus, the problem is reduced to the simultaneous solution of the system of differential equations in the partial derivatives (1) and (18) with the boundary conditions (2) – (4), (19), (20), (24). The boundary conditions are given on the boundary of the region D as well as inside it.

The conditions obtained are necessary. The question of knowing whether they are also sufficient must be resolved in each concrete case from the physical meaning of the problem.

In order to avoid solving a rather difficult boundary value problem for systems of partial differential equations, we shall proceed as follows.

We shall vary only one of the functions $x_i\,(l_\alpha + 0,\,t)$, for instance $x_k\,(l_\gamma,\,t) = x_{k\gamma}\,(t)$, in its variable $\delta x_{k\gamma}\,(t)$. We define the problem of finding an expression yielding an easy computation of the variations of the functional (5).

Since, only $x_{k\gamma}\,(t)$, varies

$$\delta x_i\,(l_\alpha + 0,\,t) = \begin{cases} \delta x_k\,(l_\gamma + 0,\,t), & i = k,\ \alpha = \gamma \\ 0, & i \neq k \quad \text{or} \quad \alpha \neq \gamma \end{cases} \quad (25)$$

must be introduced into expression (23).

The variation has an effect on the subsequent state only, but not on the preceding; therefore $\delta x_i\,(l_\alpha - 0,\,t) = 0$ for $\alpha \leqslant \gamma$.

Whereupon formula (23) becomes

$$\delta I = \sum_{i=n_1}^{n}\int_0^T \sum_{\alpha=\gamma+1}^{r-1} \delta x_i\,(l_\alpha - 0,\,t)\,\lambda_i\,(l_\alpha,\,t)\,dt - \int_0^T \delta x_k\,(l_\gamma + 0,\,t)\,\lambda_k\,(l_\gamma,\,t)\,dt \quad (26)$$

Similarly, it is not practical to use formula (26) to calculate the variation: In that case it would be necessary to find the variations $\delta x_i\,(l_\alpha - 0,\,t)$ $(\alpha = \gamma + 1,\ldots, r-1)$.Thus, we shall use a slightly different method. We shall introduce the new variables $v_{i\alpha}(t)$ in the following manner :

$$v_{i\alpha}\,(t) = x_i\,(l_\alpha + 0,\,t) - x_i\,(l_\alpha - 0,\,t), \quad v_{i0}\,(t) = x_i\,(l_0,\,t) \quad (27)$$

$$(\alpha = 1,\ldots, r-1;\; i = n_1,\ldots, n)$$

and we shall search not for the $x_i\ (l_\alpha + 0, t)$, but for the variables $v_{i\alpha}\ (t)$. It can be easily seen that if the $v_{i\alpha}\ (t)$, are known, then the quantities $x_i\ (l_\alpha + 0, t)$, can be determined with the help of (27), and vice versa (the system (1) must be solved once in that case).

From (27) we get

$$\delta x_i\ (l_\alpha + 0, t) - \delta x_i\ (l_\alpha - 0, t) = \delta v_{i\alpha}\ (t) \tag{28}$$

Substituting (28) into (23)

$$\delta I = - \sum_{i=n_1}^{n} \int_0^T \sum_{\alpha=0}^{r-1} \lambda_i\ (l_\alpha,\ t)\ \delta v_{i\alpha} dt \tag{29}$$

The variables $v_{i\alpha}\ (t)$ are independent, therefore, if only the variable $v_{k\gamma}\ (t)$ is varied then $\delta v_{i\alpha} = 0\ (i \neq k$ or $\alpha \neq \gamma)$. This yields

$$\delta I = - \int_0^T \lambda_k\ (l_\gamma,\ t)\ \delta v_{k\gamma}\, dt \tag{30}$$

We shall now consider the optimum problem having a finite number of variables. For this purpose, we shall divide the interval $[O,\ T]$ into s parts with the numbers $t_1, \ldots, t_{s-1}$. We shall assume that M is chosen sufficiently large and that all functions $v_{i\alpha}\ (t)$ are approximated by piecewise constant functions which are equal to $v_{i\alpha}^q$ inside the intervals $[t_q,\ t_{q+1}]$. The quantity I is now a function of the finite number $((n - n_1 + 1)\ rs)$ of the variables $v_{i\alpha}^q\quad (\alpha = 0, \ldots, r - 1;\ i = n_1, \ldots, n;\ q = 0, \ldots, s - 1)$

$$I_1 = I_1(v_{i\alpha}^q) \tag{31}$$

and it can be maximized by the methods of nonlinear programming. If, for instance, the gradient method is used, the successive approximations of the required quantities $v_{i\alpha}^q$ are calculated according to the formula [6]

$$(v_{i\alpha}^q)^{j+1} = (v_{i\alpha}^q)^j + h \frac{\partial I_1}{\partial v_{i\alpha}^q} \tag{32}$$

where j is the number of the iteration.

This requires the calculation of all derivatives

$$\frac{\partial I_1}{\partial v_{i\alpha}^q} \qquad (\alpha = 0, \ldots, r - 1;\ i = n_1, \ldots, n;\ q = 0, \ldots, s - 1)$$

at each iteration. Using (30), we shall find a convenient formula for the calculation of these derivatives. For this purpose, we shall vary the ordinates $v_{k\gamma}^q$ by $\delta v_{k\gamma}^q$. From formula (30) we get

$$\delta I = - \int_{t_q}^{t_{q+1}} \lambda_k\ (l_\gamma,\ t)\ \delta v_{k\gamma}^q\, dt \tag{33}$$

whereupon, since $\delta v_{k\gamma}^q =$ constant for $t_q \leqslant t \leqslant t_{q+1}$, we can easily obtain the following expression for the derivative

$$\frac{\partial I}{\partial v_{k\gamma}^q} = \frac{\delta I}{\delta v_{k\gamma}^q} = - \int_{t_q}^{t_{q+1}} \lambda_k\ (l_\gamma,\ t)\ dt \qquad \begin{pmatrix} \gamma = 0, \ldots, r - 1 \\ k = n_1, \ldots, n \\ q = 0, \ldots, s - 1 \end{pmatrix} \tag{34}$$

Thus, in order to obtain all the derivatives for the iteration, it is necessary to proceed as follows:

1. Solve the system (1) in the region D with the boundary conditions (2) – (4) and

$$x_i(l_\alpha + 0, t) = [x_i(l_\alpha + 0, t)]^j \qquad (\alpha = 1, \ldots, r-1;\ i = n_1, \ldots, n)$$

where the index j is the number of the iteration, and the $[x_i(l_\alpha + 0, t)]^j$ are the values of the controlling functions obtained for the previous iteration.

2. Store the values found for $x_i(l, t)$, $y_j(l, t)$ for a sufficiently large number of points of the region D.

3. Solve the system (18) with the boundary conditions (19) and (20), by using the stored values of $x_i(l, t)$, $y_j(l, t)$.

4. Calculate at the same time as the solution of the system (18) the values of the derivatives $\partial I / \partial v_{k\gamma}^q$ by using formula (34).

Thus, in order to make one iteration, it is necessary to solve system (1) once and system (18) once.

We note that for the system (1) the boundary conditions are given only on the segments l = const and t = const. Thus, its solution will not present any important difficulties, for instance by using the straight lines method.

The same applies also to the system (19); however, for its solution we shall move 'backwards' on both coordinates, from $l = l_r$ to $l = l_0$ and from $t = T$ to $t = 0$.

The realization of the iteration by formulas (32) guarantees the convergence of the sequence of approximations, at least to a local maximum.

In the case in which the presence of a few local maxima is assumed, the global maximum can be sought with effectiveness by using one of the global methods of search [7], since the most difficult part of these methods consists in the computation of the components of the optimized functions gradient.

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