APPLICATION OF MAXIMUM PRINCIPLE FOR OPTIMIZATION OF PSEUDO-STATIONARY CATALYTIC PROCESSES WITH CHANGING ACTIVITY

V.I. Bykov, G.S. Yablonskii, M.G. Slin'ko

Institute of Catalysis
Siberian Branch of the USSR Academy of Sciences
630090, Novosibirsk 90, USSR

The experience of using the necessary conditions of optimality in the form of L.S. Pontryagin's maximum principle for qualitative investigation and numerical calculations of optimal control for the distributed-parameter systems is discussed in the paper. Such sets of equations describe the widespread in industry class of pseudo-stationary processes with changing catalyst activity. A conception of non-local optimal control is introduced and also numerical algorithm is proposed. This algorithm allows the conditions of maximum principle to be realized on a computer.

Statement of a problem, optimality conditions. Initial equations are:

$$\frac{\partial C}{\partial \tau} = f(C,\theta,U), \qquad 0 \leq \tau \leq \tau_k,$$
$$\frac{\partial \theta}{\partial t} = g(C,\theta,U), \qquad 0 \leq t \leq t_k, \tag{I}$$

with boundary conditions:

$$C(0,t) = C^{\circ}(t), \qquad 0 \leq t \leq t_k,$$
$$\theta(\tau,0) = \theta^{\circ}(\tau), \qquad 0 \leq \tau \leq \tau_k, \tag{2}$$

where C is n-vector-function, which charactirizes the state of the process (concentrations, temperature, pressure in a reactor), m-vector-function Θ describes change of catalytic activity, t is astronomic time, τ is contact time, piecewise-continuous vector-function U characterizes control influence, its separate components being able to depend on τ or t or both τ and t; f, g are supposed to have sufficiently smooth arguments. Denote as D the field of changing independent variables τ, t, given by inequality (I).

The field of permissible controls is given in the form

$$\Omega = \left\{ U_* \leqslant U \leqslant U^* \right\} , \tag{3}$$

where U_*, U^* are constant vectors. Inequality (3) is by component one. Criterion of optimality can be presented in the most cases as follows

$$\max_{U \in \Omega} \left\{ J = \int_0^{t_k} \int_0^{\tau_k} G(C, \Theta, U)\, d\tau\, dt \right\} . \tag{4}$$

Pontryagin's maximum principle gives necessary conditions of optimality which are formulated for our case as follows /1-3/ : it is necessary for optimal control $U(\tau, t)$ in the sense of problem (I-4) that there exist such non-zero vector-functions Ψ and χ which satisfy the set of equations in D:

$$\frac{\partial \Psi_i}{\partial \tau} = -\frac{\partial G}{\partial C_i} - \left(\Psi, \frac{\partial f}{\partial C_i}\right) - \left(\chi, \frac{\partial g}{\partial C_i}\right) , \quad i = 1, 2, \ldots, n, \tag{5}$$

$$\frac{\partial \chi_j}{\partial t} = -\frac{\partial G}{\partial \Theta_j} - \left(\Psi, \frac{\partial f}{\partial \Theta_j}\right) - \left(\chi, \frac{\partial g}{\partial \Theta_j}\right) , \quad j = 1, 2, \ldots, m,$$

with boundary conditions:

$$\Psi_i(\tau_k, t) = \chi_j(\tau, t_k) = 0, \quad i, j = 1, 2, \ldots, n; m, \tag{6}$$

that on $U_k(\tau, t)$ $\forall (\tau, t) \in D$ function

$$H = G + (f, \Psi) + (g, \chi) \tag{7}$$

reaches its maximum as function of variable $U_k \in \Omega$.

Qualitative investigations. On the basis of maximum principle it is possible for some cases to carry out an investigation of optimal solutions, determine their properties of common character, obtain a priori estimations /4a-5/ . In addition the knowledge of qualitative picture of optimal strategy facilitates the choice of initial approximation already close to optimal one /4b,6/ when realizing the maximum principle as a numerical algorithm.

Let $U_{t_*}(\tau,t)$ and $U_{t_k}(\tau,t)$ be optimal controls on the segments $[0, t_*]$ and $[0, t_k]$ respectivly at $\tau \in [0, \tau_k]$, then the optimal regime is called to be local, if

$$\forall\ t_* \in (0,\ t_k) \qquad U_{t_*}(\tau,t) \equiv U_{t_k}(\tau,t).$$

Non-locality of optimal control means that the control depends on a strategy during the whole cycle at each moment and varies with changing t_k. In chemical technology such regimes are conditioned ones /3/. For optimization problem of catalytic processes with changing activity it was shown /4a/ that optimal temperature regimes were non-local ones in time, excluding only limit permissible isothermal regimes. From this fact it is clear that from a given class of problems, application of algorithm of optimal control by determination of optimal regime for stationary conditions is invalid . In addition, for non-local control it is necessary to take strictly into account the limitations on control parameters. Imposition of limitations after calculation of the controls can lead to considerable mistakes in given case /3/.

An example of a problem of singular control that arises for considered class of optimization problems (I-4) can be the problem of cooler optimal temperature determination T_x in tube reactor with cooling and decaying catalyst activity:

$$\frac{\partial C}{\partial \tau} = f_1(C,\theta,T), \qquad \frac{\partial \theta}{\partial t} = g(C,\theta,T), \tag{8}$$

$$\frac{\partial T}{\partial \tau} = f_2(C,\theta,T) - B(T - T_x), \tag{9}$$

where

$$T_{x*} \leq T_x(\tau, t) \leq T_x^*$$

and it is required to obtain

$$\max \int_0^{t_k} C(\tau_k, t)\,dt \ . \qquad (10)$$

Control T_x goes to (9) in a linear form and that is why it **may** have singular sections. The difficulty of singular control determination here can be overcome in the following way. Optimal temperature profile $T(\tau, t)$ is determined by carriying out the stage of theoretical optimization, that is by solution of the problem (8), (10) with control T. Substituting $T(\tau, t)$ in thermal balance equation (9) we obtain T_x :

$$T_x = T + \frac{1}{B}\left[\frac{\partial T}{\partial \tau} - f_2(\tau, t)\right] \quad ,$$

which is optimal singular control after satisfying given limitations.

Numerical algorithm. Necessary conditions of optimality in the form of maximum principle make up the boundary problem (1,2,5,6) where the controls at each point of D are determined from H function maximum condition, H being known from (7). Boundary problem as stated here in operator form can be written as follows

$$\mathscr{D}X + F(X, U_{opt.}) = 0 \ , \qquad (11)$$

where vector of optimal controls $U_{opt.}$ is determined from condition

$$H(X, U_{opt.}) = \max_{U \in \Omega} H(X, U) \ .$$

Side by side with (11) consider a set of equations

$$\frac{\partial Y}{\partial \xi} = \mathscr{D}Y + F(Y, U_{opt.}) \ , \quad Y\big|_{\xi=0} = Y^o , \qquad (12)$$

with boundary conditions (2,6). If $Y(\xi, t, \tau) \rightarrow X(\tau, t)$ at $\xi \rightarrow \infty$, (that is solution of the problem (12) converges to solution of (11) at the same boundary conditions irrespective of initial data choice) then sought-for optimal control can be found by realization on computer of the difference scheme approximating equations (12).

The algorithm proposed was used for optimal temperature determination for different schemes of reactions in plug flow and incomplete mixing reactors. Convergence was observed in all considered cases after50-60 iterations. The required computing time decreased by a factor of 5-10 as compared to the trial and error method /7/. Algorithm can easily be generalized also for the problems of terminal control.

The solution of a number of optimization problems of important industrial processes with decaying catalyst activity /5,6/ can state that apparatus of maximum principle gives not only possibility to carry out qualitative investigation of optimal control, but also on its basis to build effective calculative algorithms for seeking optimal conditions to conduct a class of catalytic processes.

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