TO THE PROBLEM OF OPTIMIZATION OF INDUSTRIAL PETROCHEMICAL REACTORS

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1. Introduction. The problem of optimization of industrial petrochemical reactors as systems with distributed parameters is interesting not only from positions of problems of control, but also from more common positions, including problems of optimum hardware registration. The solution of this problem emerges from the search for an optimum theoretical mode, which can facilitate the choice of a design of the technological apparatus and computation of the control strategy of a concrete petrochemical reactor.

2. The problem. In this work the problem of optimization of one class of non-stationary petrochemical reactors with distributed parameters is considered. Experience of application of necessary optimality conditions in the form of Pontryagin's maximum principle and the computational side of the problem are discussed. In particular, the efficiency of approaches based on direct variation methods is discussed.

3. Solution methods. *The initial equations*. The mathematical model of considered processes is represented by the differential equations of the following kind:

$$\frac{\partial C}{\partial x} = f(C,S,U), \quad 0 \le x \le 1 , \quad \frac{\partial S}{\partial t} = g(C,S,U) , \quad 0 \le t \le 1 , \tag{1}$$

with boundary and initial conditions:

$$C(0,t) = C^o(t), \quad 0 \le t \le 1, \quad S(x,0) = S^o(x), \quad 0 \le x \le 1, \tag{2}$$

Where the vector *C* characterizes the condition of the process (concentration of reagents, temperature) distributed on space coordinate *x*; vector S reflects the change of the process in time *t* and characterizes intensity of the process (the degree of activity of the catalyst); the vector of piecewise-continuous functions *U* indicates controlling influence. Separate components *of U* can depend on *x* or *t*, or on both variables *x*, *t*. As a mean of control $C^o(t)$, $S^o(x)$ can also act. Restrictions on control are usually set as coordinate-wise inequalities; the optimality criterion means the requirement:

$$\max_{u \in U} \int_0^1 \sum q_i C_i(1,t)dt , \tag{3}$$

Where U is the area of allowable controls, factors q_i are cost parameters and reflect component-wise value of the reacted mix in the output from the reactor.

Optimality problems such as (1-3) arise, for example, during control of a petrochemical reactor with a motionless layer of the catalyst characterized by falling of activity in time. Experience of the solving of similar tasks shows that it is expedient to solve them in two stages. The first is a theoretical optimization which is carried out on the basis of kinetic model of the process. After solving this problem the technological circuit of contact unit is chosen which allows getting closer to a theoretical mode in the best way. The second stage is the actual optimization or calculation of optimum control for the chosen type of a reactor. It is necessary to note that in industry due to limited metrological characteristics of the technical means of the control and specifics of regulators controlling parameters may vary only in steps as partly-constant function.

Theoretical optimization. Necessary conditions of an optimality for the formulated problem (1-3) can be written down in the form similar to Pontryagin's principle of maximum [1] . Here the concept of non-locality of optimum strategy is essential. Let *u (t)* and *u * (t)* be optimum in the connect of (1-3), on [0,1] and [0, t_*], $0 \le t_* \le 1$, accordingly . Then we shall name the optimum strategy local if $\forall t_* \in [0,1]$ $u^*(t) \equiv u(t),\ t \in [0, t_*]$, also non-local, otherwise. For the control which depends on two variables, it is possible to speak about locality of control on corresponding variable. In the case of non-locality of the optimum strategy the application of search algorithms of optimum control by optimization at each moment of time is impossible. Realizations of the principle of maximum yields the necessity to solve a boundary problem.. Besides, there are restrictions on u for non-local control. Their application after all calculations is no more feasible. For the problem of theoretical optimization of catalytic process with falling activity, the temperature mode $(u = T(x,t), (u = T(x,t),$ is the control, and the maximum output of the final product ($max \int_0^1 c_ц(1,t)dt$) is the criterion. Here on the basis of necessary conditions of optimality in the form of a maximum principle it is proved [1], that optimum temperature modes are not local (maximum permissible isothermal modes $T \equiv T_{max}$ are the exceptions).

Let's consider the system of the equations representing mathematical model of process of transformation $A \rightarrow B$ in view of falling of activity of the catalyst.

$$\frac{\partial c}{\partial x} = -k_1(T)cs,\ c(0,t) = 1,\ 0 \le t \le 1, \qquad \frac{\partial s}{\partial t} = -k_2(T)cs,\ s(x,0) = 1,\ 0 \le x \le 1,$$

Where $k_i(T) = k_i^o \exp(-E_i / RT),\ \ i = 1,2$,

Restrictions in the form of bilateral inequalities $T_{min} \le T(x,t) \le T_{max}$. are imposed on the temperature *T (x, t)*. It is required to find such piecewise-continuous *T (x, t)* that ensures that $min \int_0^1 c(1,t)dt$. is reached. It is essential to single out two cases:

1. $E_1 < E_2$. Then the temperature determined on the basis of maximum of Hamiltonian, can lay inside the accessible region and can be laid out as:

$$T = (E_2 - E_1)/R \cdot ln \frac{k_2 E_2 |\psi_2|}{k_1 E_1 \psi_1},$$

Where $\psi_1, \psi_2 -$are corresponding conjugate functions. The analysis of transvensality conditions allows to draw a conclusion, that the optimum temperature during the final moment of time accepts as the maximum possible value $T(x,1) \equiv T_{max}$. Further, if the condition $\alpha \exp(\alpha + \beta) \le E_1 / E_2,\ \alpha = k_2(T_{max}),\ \beta = k_1(T_{min}),$ is satisfied, then $T(x,t) = T_{max}$. However if $exp(2\beta) \le \gamma E_2 / E_1,\ \ \gamma = k_2(T_{min}),$ then optimum $T(x,t)$ inside the set area of change of independent variables *D* accepts value T_{min}.

2. $E_1 > E_2$. The optimum temperature has relay character, i.e. accepts only boundary allowable values. The conditions similar to the previous can exist in this case, too.

If $\gamma \exp(\alpha + \beta) \le aE_1 / E_2,\ \ a = k_1(T_{min}),$ then in area D the optimum temperature is $T(x,t) \equiv T_{max}$. The condition of existence in area D of switching of optimum temperature from T_{min} to T_{max} is contained in the statement: if $exp(2\beta) \le a\gamma E_2 / E_1$, then the optimum $T(x,t)$ inside D accepts value T_{min}. The basic conclusion of the analysis of influence of parameters of a problem on the kind of optimum control is contained in the statement: the structure of optimum temperature is determined by the correlation of E_1 and E_2: at $E_1 > E_2$ the control is all-relay, at $E_1<E_2$ a curvilinear area can exist in the form of a function monotonously growing in time.

Thus, on the basis of the maximum principle it is sometimes possible to carry out a qualitative research of optimum decisions, to reveal their general properties, to understand the structure of the optimum mode, to get some *a priori* estimates. Besides, the knowledge of the qualitative picture of optimum strategy by numerical search for optimum control facilitates the choice of the initial approximation, which is already close enough to optimum.

Computing aspect. For the considered class of problems of optimization, the development or a choice of effective numerical algorithm and its substantiation is especially important.

For the solution of considered problems numerical definition of optimum controls can be carried out on the basis of application of various methods, however the maximum principle is applied most frequently. The discussion of experience of use of necessary conditions of optimality in the form of maximum principle, and the computing side of the problem is deemed expedient.

Generally among controls there can be vector functions both of two $T(\tau,t)$, and one variable $m(t)$. Boundary conditions $C^0,\ \theta^0$ can also be controlled. When optimizing the mode of a reactor it is enough to add the equations of thermal balance to system (1) and add in the temperature $T(\tau,t)$ to the components of the vector $C_i(\tau,t)$, to receive model of the reactor. The problem of optimization is reduced to determinations of controls from the condition of an extremum of function H which is generally found using methods of nonlinear programming.

The solution of the boundary problem for control systems of various structures is difficult enough and labour-intensive computing task. In the latter case it is necessary to solve a boundary problem for the system of the initial and conjugate equations with the feature, that in real-life problems the right parts of the equations are often complex functions of state variables of, and their analytical differentiation for finding systems of conjugate equations can appear quite labour-intensive. Numerical differentiation demands the constant control of accuracy, otherwise it can lead to significant errors. The difficulties with construction of computing circuits on the basis of maximum principle can be fundamental in nature. In the case of the non-linear equations the dependence on initial conditions of potentially optimum controls is complex. Therefore iterative search methods of the optimum control, based on a principle of a maximum, do not often converge. Even in case of convergence there is no guarantee, that the found control delivers a global maximum of the functional. Theoretically it is possible to add a possibility of existence of special controls to difficulties of use of the maximum principle.

At the same time, as it has been demonstrated, on the basis of the maximum principle, besides getting the quantitative results, sometimes it is possible to make qualitative researches of optimum decisions, to reveal their general properties, to understand the structure of optimum decisions, to get some a priori estimations [1]. Besides, the knowledge of qualitative picture of optimum strategy when performing numerical search for optimum control facilitates a choice of initial approximations, already close enough to optimum.

General shortcoming of this and many other iterative methods of optimization in cases of nonlinear controls and nonlinear functional, is the locality of obtained results, as discovery of only the local extremum is guaranteed. Their application is even more complicated when searching for optimum values of control as step function. In this case the solution of the problem is complicated manifold, partially due to complexity of the equations of the conjugate system.

For such problems the most effective approach is the application of the direct variation methods which do not use necessary conditions of an extremum directly, and are reduced to integration of the basic system of the equations with an added method of search for an extremum of corresponding functional. Direct methods of the decision of variational problems differ in ways of construction of minimizing sequences.

Numerical realization of direct methods has shown that with their help one can find controls giving the function being minimized the values close enough to the extreme one.

However, the controls received can differ significantly from optimum control [2]. The practice of optimization calculations has shown, that for an establishment of globality of an extremum of the target function the search of unknown factors of decomposition of the equations of basic functions should be repeated with various initial estimations. Besides, the search was complicated by strong mutual influence of factors. Various restrictions on controls and phase variables can be taken into account with the help of penalty functions. The initial problem is reduced by application of direct methods to some finite-dimensional one, for which with the help of methods of nonlinear programming the problem of finding of optimum values of controls and parameters τ_k, t_k is solved. At known structure of optimum control the application of direct methods does not present difficulties. If the structure is unknown, reducing the function of the initial problem to functions with consecutive inclusion of unknown values, by application of a method of local variations the independent variation of a separate small piece of the trajectory is reached [3].

At the same time it is necessary to take into account, that at designing new processes, as a rule, a priori data on the structure of the optimum temperature mode is absent.

Experience of use of direct methods for determination of the optimum temperature structure $T(\tau)$ shows, that efficiency of their application is related to the kind of circuits of reactions. Depending on complexity, branching of chemical reactions, application of discrete variants of the direct methods using a variation in space of controls, Ritz method, or the modified procedure of a method of local variations become effective in practice [2].

In problems of determination of theoretical optimum mode, at two-dimensional distribution of controls, application of direct methods is limited to difficulties of approximation of multivariate functions.

4. Conclusions. In real problems controlling influences of chemical reactors, as a rule, are functions of one variable. Therefore it seems that when solving problems of optimization of industrial non-stationary petrochemical processes, including catalytic ones, the direct variation methods significantly simplifying the search of one-dimensional optimum controls, should be increasingly applied.

Literature

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