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Solving the Optimal Control Problem with Terminal Constraints in Modeling Chemical Processes

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Abstract

The paper presents a method for solving the problem of optimal control of a chemical process in the presence of terminal constraints based on the application of artificial immune systems. The formulation of the problem of optimal control of a chemical process in which the constraints on the control parameter and phase variables are given is formulated. An algorithm for solving this problem based on the penalty method and artificial immune systems is given. The penalty method allows to reduce the problem with terminal constraints to the problem without constraints by changing the optimality criterion. The new optimal control problem without

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terminal constraints is solved by the method of artificial immune systems. The described methodology is tested on the example of an industrially significant process of phthalic anhydride production. A mathematical description of the process, which is a system of ordinary differential equations, is given. The problem of search of optimal temperature regime with terminal constraints is formulated. As a result of calculations, the optimal temperature regime and the corresponding optimal concentrations of substances are determined. At the same time, the restrictions on the concentration value of the reaction by-product and the conversion of substances at the end of the reaction are fulfilled. It is shown that the solution of the optimal control problem with terminal constraints for the process of phthalic anhydride production satisfies the constraints of the problem and provides the highest value of the concentration of the target reaction product.

1 Introduction

The main task of functioning of an industrial enterprise is to maximize the efficient use of available resources with minimal production costs. This problem can be solved by using digital twins of chemical-technological processes, including specialized software that allows to simulate the operation of the technological plant.

Among the problems of mathematical modeling of chemical processes, optimal control problems are of greatest practical interest. To formalize the problem of searching for optimal mode parameters of a chemical process, it is necessary to compile its mathematical model (for example, in the form of a system of differential equations), to identify the control parameters and the area of their variation, and to designate the criterion of control quality.

Currently, there is a large number of works on the problems of control of dynamic systems [1–10].

In optimal control problems, restrictions can be imposed not only on control parameters, but also on phase variables If the constraints on phase variables are set at a finite moment of time of system operation, then such a problem is a problem with terminal constraints. The development of numerical methods for solving the optimal control problem with terminal constraints is of scientific and practical interest. More complex problems with phase and intermediate constraints can be reduced to terminal problems by applying mathematical reductions.

There are several approaches for solving optimal control problems with phase constraints. One of them assumes the derivation of exact optimality conditions and the study of properties of the obtained solutions [11, 12]. The necessary conditions of optimality of solutions of optimal control problems with phase constraints in the form of Pontryagin's maximum principle are obtained in [13, 14]. However, when developing numerical algorithms for solving optimal control problems, this approach is difficult to implement in practice.

Another approach involves reducing the problem with terminal constraints to a problem without constraints by applying the penalty method. In this method, an auxiliary optimality criterion containing a penalty functional for violation of the phase constraints is introduced. Then the problem of optimal control without constraints is solved, in which the auxiliary functional is a criterion of control quality.

A number of works are devoted to the development of methods for solving optimal control problems with terminal constraints based on the penalty method [15–19]. Numerical realization of this method is presented in [20, 21]. A sequence of optimization problems without constraints is solved using the gradient method. The sensitivity of the solution of the optimization problem to the choice of the initial approximation is a disadvantage of gradient methods. This can lead to the solution falling into a local extremum or into a region that contradicts the physical meaning of the problem.

Most numerical methods for solving optimization problems encounter a number of difficulties during their software implementation. These difficulties are related to the nonlinearity of the model describing the chemical process, the high dimensionality of the problems to be solved, the presence of phase constraints, and the sensitivity of the solution found to the initial search point [22, 23]. The application of evolutionary optimization methods allows us to overcome the above mentioned difficulties. The method of artificial immune systems is one of the evolutionary methods.

The method of artificial immune systems is based on imitating the functioning of the immune system of living organisms, which is to protect against unfavorable external influences (pathogens, antigens) [24–28]. The main role is played by defense cells - antibodies produced by immune cells. Antibodies undergo changes in the course of the fight against antigens and pathogens. The antibodies most adapted for defense inhibit foreign bodies. The immune system memorizes these antibodies to reproduce them when the body is attacked again by a similar pathogen.

The important advantages of the method of artificial immune systems are the independence of the solution of the optimization problem from the initial approximation, as well as the absence of the requirement for continuity of the target function and its derivatives. The lack of sensitivity of the solution to the initial approximation is achieved due to the fact that at the beginning of the search a set of vectors of possible solutions are specified. The vectors are filled with random admissible values. Then they undergo changes by applying the method operators, approaching the solution of the optimization problem. Compared to other evolutionary methods, artificial immune systems operate in their work with the best solutions found in the previous iteration of the search. This allows their application in solving multimodal optimization problems.

The method of artificial immune systems is used to solve optimization and optimal control problems. In [29, 30], solutions of optimization problems in power engineering and power systems based on the method of artificial immune systems are presented. In [31,32] the application of artificial immune system for solving optimization problems of multimodal functions is considered. The work [33] describes immune methods for solving the main types of optimization problems: unconstrained problem, constrained problem, multimodal problem and multicriteria problem.

In [34] the problem of finding suboptimal program control for continuous deterministic systems is considered. The problem contains constraints on the control parameter and does not contain phase constraints. For its solution, an algorithm based on the method of artificial immune systems is given.

The studies mainly consider optimization problems of functions. Significantly fewer works are devoted to the solution of optimal control problems. The actual problem is the development of an algorithm for solving the optimal control problem with constraints imposed on phase variables.

This paper presents a step-by-step algorithm for finding a numerical solution to the problem of optimal control of a chemical process with terminal constraints.

2 Materials and methods

Let the dynamics of the chemical process be described by a system of ordinary differential equations [35]

$$\frac{dx}{dt} = f(t, x(t), u(t)) \tag{1}$$

with initial conditions

$$x(0) = x^0, \tag{2}$$

where $x(t) = (x_1(t), x_2(t), ..., x_n(t))^T$ – vector of phase variables, $u(t) \in U$– control parameter, U – set of admissible control values, $t \in [0, t_1]$ – time, $f(x(t), u(t), t) = (f_1(x(t), u(t), t), f_2(x(t), u(t), t), ..., f_n(x(t), u(t), t))^T$ – vector function continuous together with its partial derivatives.

The control parameter $u(t)$ can be temperature, pressure, feed rate of the reaction mixture, etc.

Let the set U be given by the inequality:

$$u_a \le u(t) \le u_b, \quad t \in [0, t_1], \tag{3}$$

where u_a, u_b are upper and lower permissible bounds of the control parameter values.

Let the constraints be imposed on the phase variables at time t_1:

$$r_j(x(t_1)) = 0, \quad j = \overline{1, m}, \tag{4}$$

$$r_j(x(t_1)) \le 0, \quad j = \overline{m+1, p}, \tag{5}$$

where $r_j(x)$ are continuous-differentiable functions.

Let's introduce the control quality functional:

$$R(u) = r_0(x(t_1)) \to \min. \tag{6}$$

It is required to find a control function $u^*(t) \in U$ satisfying constraints (4), (5), for which the optimality criterion (6) takes the minimum value.

We apply the penalty method and the method of artificial immune systems to solve the optimal control problem (1)–(6).

The main idea of the penalty method is to construct a new optimality criterion with a penalty functional $W(u, s^k)$. The value of the penalty functional is equal to zero when constraints (4), (5) are satisfied, and greater than zero otherwise. Therefore, let us consider the optimality criterion

$$P(u) = R(u) + W(u, s^k) \to \min, \tag{7}$$

where $W(u, s^k)$ – penalty functional defined by the formula

$$W(u, s^k) = \frac{s^k}{2} \left(\sum_{j=1}^{m} |r_j(x(t_1))|^2 + \sum_{j=m+1}^{p} (max\{0, r_j(x(t_1))\})^2 \right),$$

k – iteration number, s^k – penalty parameter.

It is necessary to find a solution to the optimal control problem without constraints at each iteration of the solution search. The found control parameter $u^*(t)$ becomes the initial one for the next iteration with an increased value of the penalty parameter.

The sequence of solutions to the optimal control problem (1)–(3), (7) gives the solution to the original problem (1)–(6).

We apply the method of artificial immune systems to solve the problem of optimal control (1)–(3), (7). The optimality criterion (7) expresses the adaptability of the immune cell to the fight against foreign bodies. The optimality criterion is a fitness function. Let the immune cell be the vector of control parameters $u = (u_1, u_2, ..., u_l)$, and the set of such vectors constitutes a population:

$$u^i = (u_1^i, u_2^i, ..., u_l^i), \quad i = \overline{1, count\_u}. \tag{8}$$

The most adapted immune cell u corresponds to the smallest value of the fitness function (7), since the problem of finding the minimum of the optimality criterion is being solved.

Let us formulate a numerical algorithm for solving the optimal control problem with terminal constraints.

1. Set the parameters of the artificial immune systems algorithm: initial value of the penalty parameter s^0, population size $count\_u$, number of immune cells with the worst fitness function value $maxf$, number of parent cells for selection sel, number of clones for the cloning operator $klon$, mutation operator parameter mut, solution search termination parameters ε_1, ε_2.

2. Fill the initial population of immune cells (8) with acceptable values from the U region randomly.

3. Compute the value of the fitness function (7) for each immune cell u_i, $i = \overline{1, count\_u}$.

4. Apply the cloning operator to the current population. Select the most adapted immune cells (parent cells) and create $klon$ copies for each cell.

5. Apply the mutation operator to each clone vector. Generate random numbers $q_1 \in [0, u_b - u_j^i]$, $q_2 \in [0, u_j^i - u_a]$, $q_3 \in [0, 1]$ for each parent cell. The parameter q_3 is the probability. Depending on the value of q_3 (greater or less than 0.5), the value of the clone coordinate is calculated by the first or the second line of the formula:

$$u_{mut}^i = \begin{cases} u_j^i + q_1 \cdot mut, & q_3 > 0.5, \\ u_j^i - q_2 \cdot mut, & q_3 \leq 0.5. \end{cases}$$

6. Calculate the value of the fitness function (7) for each mutant cell.

7. Apply the selection operator to each mutant clone. Select the most adapted cells among them. Place them in the population instead of the parent cell, provided that it is less adapted than the mutant clone.

8. Generate $maxf$ new immune cells randomly. Calculate the fitness function value for them.

9. Select $maxf$ least adapted immune cells from the population. Replace them with new cells.

10. Check the termination condition for finding a solution to the optimal control problem without constraints.If the change of the fitness function value does not exceed the given small value ε_1, then select the cell u^* with the smallest fitness function value from the last population. Otherwise, proceed to step 4.

11. Check the termination condition of the algorithm. If $W(u^*, s^k) > \varepsilon_2$, then increase the penalty by the rule:

$$s^{k+1} = 10 \cdot s^k.$$

Set the best adapted immune cell u^* as the initial population for the next iteration of the algorithm. Then proceed to step 4.

If $W(u^*, s^k) \leq \varepsilon_2$, then stop the algorithm. The most adapted immune cell u^* from the last population is the solution to the optimal control problem.

3 Research results

Let us find a numerical solution of the optimal control problem with terminal constraints for an industrially significant process of phthalic anhydride production using the described method. Phthalic anhydride is used in the production of paint and varnish products, medicines, plasticizers, dyes, additives to lubricating oils and others. The scheme of chemical reaction of phthalic anhydride production is described by the following set of stages [36]:

$$\begin{aligned} X_1 &\to X_2, \\ X_2 &\to X_4, \\ X_1 &\to X_3, \\ X_1 &\to X_4, \\ X_2 &\to X_3, \\ X_3 &\to X_5, \end{aligned}$$

where X_1 – naphthalene, X_2 – naphthoquinone, X_3 – phthalic anhydride, X_4 – carbon dioxide, X_5 – maleic anhydride.

The kinetic equations can be represented in the following form according to the law of acting masses:

$$\begin{aligned} w_1(x,T) &= k_1(T)x_1, \\ w_2(x,T) &= k_2(T)x_2, \\ w_3(x,T) &= k_3(T)x_1, \\ w_4(x,T) &= k_4(T)x_1, \\ w_5(x,T) &= k_5(T)x_2, \\ w_6(x,T) &= k_6(T)x_3, \end{aligned}$$

where $w_j(x,T)$ is the rate of the j-th reaction step ($j = \overline{1,6}$) (1/h), x_i is the concentration of the i-th substance ($i = \overline{1,5}$) (mole fraction), T – temperature (K). The rate constants of stages k_j ($j = \overline{1,6}$) (1/h) depend on temperature T based on the Arrhenius equation

$$k_j(T) = k_{0j} \exp\left(-\frac{E_j}{RT}\right),$$

where k_{0j} – pre-exponential multiplier (1/h), E_j – value of the activation energy of the j-th stage (J/mol), R – universal gas constant ($8.31 J/(mol \cdot \hat{E})$).

Numerical values of kinetic parameters of the reaction of phthalic anhydride production are given in [36].

The matrix of stoichiometric coefficients of substances of the reaction of phthalic anhydride production is given in Table 1.

Table 1. Matrix of stoichiometric coefficients

	w_1	w_2	w_3	w_4	w_5	w_6
X_1	-1	0	-1	-1	0	0
X_2	1	-1	0	0	-1	0
X_3	0	0	1	0	1	-1
X_4	0	1	0	1	0	0
X_5	0	0	0	0	0	1

Dynamics of concentrations of substances of the reaction of phthalic anhydride production is described by a system of ordinary differential equations:

$$\begin{aligned}\frac{dx_1}{dt} &= -w_1(x,T) - w_3(x,T) - w_4(x,T),\\ \frac{dx_2}{dt} &= w_1(x,T) - w_2(x,T) - w_5(x,T),\\ \frac{dx_3}{dt} &= w_3(x,T) + w_5(x,T) - w_6(x,T),\\ \frac{dx_4}{dt} &= w_2(x,T) + w_4(x,T),\\ \frac{dx_5}{dt} &= w_6(x,T),\end{aligned} \tag{9}$$

with initial conditions

$$x_i(0) = x^0, \quad i = \overline{1,5}. \tag{10}$$

Variables x_i $(i = \overline{1,5})$ (concentrations of substances) are phase variables in the system of differential equations (9). The reaction temperature T is a control parameter.

Let technological constraints be imposed on the temperature values:

$$620K \leq T \leq 644K. \tag{11}$$

Phthalic anhydride X_3 is the target product of the reaction. Therefore, we set the maximum value of phthalic anhydride concentration at the end of the reaction as an optimality criterion:

$$x_3(t_1) \to \max. \tag{12}$$

The process of formation of phthalic anhydride directly depends on the conversion of substances X_1 and X_2. Therefore, we require that the conversion of these substances is 95% at the end of the reaction:

$$1 - (x_1(t_1) + x_2(t_1)) = 0.95. \tag{13}$$

Carbon dioxide X_4 is a by-product of the reaction to produce phthalic anhydride. We add the condition that its concentration should not exceed 20% at the end of the reaction:

$$x_4(t_1) < 0.2. \tag{14}$$

Let's set the initial values of substance concentrations (in mole fractions):

$$x_1(0) = 1, \quad x_i(0) = 0, \quad i = \overline{2,5}. \tag{15}$$

The problem of optimal control of the process of phthalic anhydride production with terminal constraints is formulated as follows. It is necessary to find the optimal temperature regime $T^*(t)$, which ensures the maximum of the optimality criterion (12) with regard to the constraints (11), (13), (14).

A program has been developed in the Delphi visual programming environment to find a numerical solution to the problem of optimal control of the process of phthalic anhydride production. The process with duration $t_1 = 1$ h is considered. The Runge-Kutta method of the 4th order is applied for numerical solution of the system of differential equations (9) with initial conditions (10).

The developed algorithm is applied with the following parameters: $s^0 = 0.01$, $count\_u = 40$, $maxf = 10$, $sel = 15$, $klon = 10$, $mut = 0.5$, $\varepsilon_1 = \varepsilon_2 = 10^{-4}$.

The optimal temperature regime of the process of phthalic anhydride production and the dynamics of optimal concentrations of substances as a result of solving the optimal control problem (8)–(15) have been calculated (Fig. 1-3).

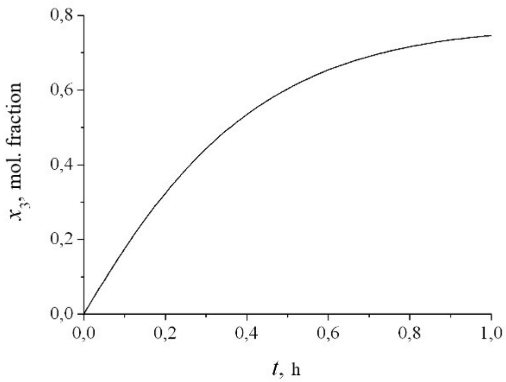

Figure 1. Dynamics of phthalic anhydride concentration X_3

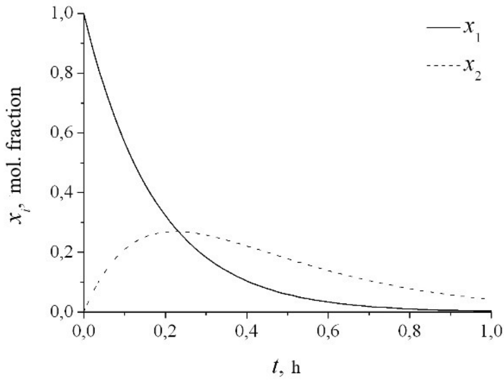

Figure 2. Dynamics of naphthalene X_1 and naphthoquinone X_2 concentrations

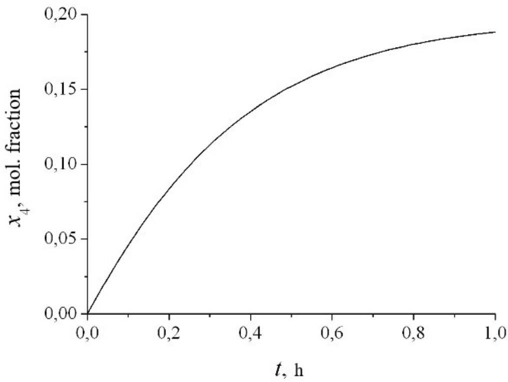

Figure 3. Dynamics of carbon dioxide concentration X_4

To achieve at the end of the reaction the maximum concentration of the target substance X_3, equal to 0.746 mole fraction, it is necessary to maintain a constant temperature $T^* = 620$ K. In this case, the conversion of X_1, X_2 will be 95.3%, and the concentration of the by-product will be equal to 0.188 mole fractions.

Fig. 1 shows the time dependence of the concentration of the target product of the reaction phthalic anhydride X_3. As can be seen from the figure, it monotonically increases throughout the entire time of the reaction.

The concentration of naphthalene X_1, shown in Fig. 2, decreases monotonically with time. This is due to the consumption of this reagent in the first, third and fourth stages of the reaction. Fig. 2 also shows the time variation of naphthoquinone concentration X_2. The concentration of this substance increases up to the time $t \approx 0.23$ h. Then until the end of the reaction there is a decrease in the concentration of naphthoquinone. This is due to the predominance of its consumption in the second and fourth stages over synthesis in the first stage.

Fig. 3 shows the dependence of carbon dioxide concentration X_4 on time, which is a monotonically increasing function. This is explained by the fact that carbon dioxide is formed from the target substance X_3 in the sixth stage, and then is not consumed.

Table 2 shows the results of calculation of optimality criterion (12), conversion of substances X_1, X_2, concentration of by-product substance X_4 at some values of permissible temperature. The table shows that the solution of the optimal control problem satisfies the constraints of the problem and provides the largest value of the concentration of the target reaction product.

Table 2. The value of terminal constraints and optimality criteria at acceptable temperature values

No.	T, K	$1-(x_1(t_1)+x_2(t_1))$, mol. fraction	$x_4(t_1)$, mol. fraction	$x_3(t_1)$, mol.fraction
1	620	0.953	0.188	0.746
2	625	0.947	0.192	0.745
3	630	0.942	0.196	0.740
4	635	0.979	0.200	0.731
5	640	0.984	0.203	0.717
6	644	0.987	0.205	0.702

4 Conclusion

The developed algorithm makes it possible to find a solution to the problem of optimal control of a chemical process in the presence of restrictions on the phase variables and on the control parameter. The operation of the algorithm is based on the application of the penalty method and artificial immune systems. Using the penalty method, the original problem with terminal constraints is reduced to an unconstrained optimal control problem, the solution of which is sought using the method of artificial immune systems. A feature of the developed algorithm for solving an optimal control problem with terminal constraints is independence from the starting point of the search for a solution.

A computational experiment was carried out for the process of obtaining phthalic anhydride based on the described method. The optimal temperature regime has been determined, which ensures the achievement of the maximum concentration of the target product - phthalic anhydride. At the same time, restrictions on the value of the concentration of the by-product of the reaction and the conversion of substances at the end of the reaction are fulfilled. It is shown that the value of the concentration of the target substance, calculated at the optimum temperature, is higher than the values of its concentrations, calculated at certain allowable temperatures, and at the same time, the terminal restrictions are observed.

Thus, the proposed method for solving the optimal control problem with terminal constraints can be used to determine the optimal parameters of chemical processes.

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