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Search for the Optimal Composition of the Reaction Mixture Based on a Genetic Algorithm

Evgenia Antipina[a], Svetlana Mustafina[a], Andrey Antipin[a], Andrey Akimov[a,*]

[a] *Ufa University of Science and Technology, st. Zaki Validi 32, 450076 Ufa, Russia*

stepashinaev@ya.ru, mustafina_sa@mail.ru, andrejantipin@ya.ru, andakm@yandex.ru

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Abstract

The problem of determination of optimal initial concentrations of catalytic reaction reagents is considered. The mathematical description of the reaction is a system of ordinary differential equations. Restrictions are imposed on the values of concentrations of substances at the initial moment of time. To find a solution to the problem, a genetic algorithm with real coding has been developed, taking into account the physical and chemical meaning of the problem. The algorithm is modified at the stage of initial population filling, crossover and mutation. The developed algorithm takes into account the constraints set on the values of initial concentrations of reagents. The work of the algorithm is tested on the example of the catalytic reaction of benzyl butyl ether synthesis. As a result of numerical experiments the initial concentrations of reagents, at which the highest values of concentrations of target products of the reaction – benzylbutyl ether and dibenzyl ether – are provided, have been calculated. The values of concentrations of target products of reaction at other initial compositions of reaction mixture have been calculated. It is shown that the set of initial concentrations

*Corresponding author.

of reagents calculated with the help of the algorithm provides the highest values of concentrations of target reaction products.

1 Introduction

At present, the use of mathematical modeling methods for chemical engineering processes allows finding solutions to a number of practical problems, one of which is determining the optimal conditions for their implementation. When studying the patterns of chemical processes, it is not always possible to conduct a sufficient number of experiments due to high costs for raw materials and equipment. Therefore, an urgent scientific task is the development of mathematical methods and algorithms that allow simulating a laboratory experiment at the stage of a computational experiment.

The kinetic model of a reaction is one of the main levels of mathematical modeling of a chemical process. It includes a list of reagents, individual stages of their transformation, an equation of the rates of stages depending on the concentrations of reagents and temperature [1]. A mathematical description of the change in concentrations of reactants over time can be presented as a system of ordinary differential equations. The initial conditions of the system determine the initial composition of the reacting mixture.

The optimized conditions for the chemical reaction can be temperature, pressure, reaction mixture composition, feed rate, process duration, etc. A practically significant task in studying chemical reactions is to predict the properties of the resulting product depending on the ratio of the concentrations of the substances that have entered into the reaction. In other words, it is necessary to determine the initial composition of the reaction system in order to ensure the maximum yield of the target reaction products, the minimum yield of by-products, to achieve a certain level of conversion of the initial substances, etc. The solution to this problem can be obtained by formalizing it based on kinetic modeling of the chemical reaction and the use of numerical optimization methods.

A number of works are devoted to solving optimization and optimal

control problems in chemistry and chemical engineering.

Pontryagin's maximum principle is widely used to find optimal control of chemical processes. The maximum principle is a fundamental concept of optimal control theory. The problem of optimal control of parallel chemical reactions is considered in [2]. Here, temperature, pressure, and reaction rate constants act as control parameters. Pontryagin's maximum principle is used to determine the optimal temperature regime of a catalytic process in a cascade of reactors in [3]. However, the application of the maximum principle requires additional verification of the found solution for optimality, which is a resource-intensive task.

Dynamic programming is used to optimize multi-stage processes in chemical engineering. The effectiveness of dynamic programming is shown in [4]. This method has proven itself in solving problems in which there is a small number of variables at each stage. However, it is not practical to use it for complex chemical reactions containing a large number of intermediate substances. In this case, the problem is high-dimensional, which leads to resource-intensive calculations.

Mathematical models of chemical processes have a number of features. These include nonlinearity, high-dimensional problem, phase constraints, etc. Therefore, computational difficulties arise in the numerical implementation of algorithms based on classical optimization methods.

The use of genetic algorithms allows us to overcome the listed disadvantages of most optimization methods. Genetic algorithms are a method of evolutionary computations. Their operation is based on the imitation of the processes of evolution of living organisms [5, 6]. A distinction is made between genetic algorithms with binary and real coding. The gene is encoded using a binary representation in genetic algorithms with binary coding. In this case, the stages of encoding and decoding the optimized process parameters are included in the algorithm. The gene is represented by a real number in genetic algorithms with real coding. Therefore, there is no need for additional operations associated with recoding [7, 8].

Currently, genetic algorithms are widely used to solve optimization problems in molecular modeling [9], multicriteria optimization [10], to solve planning problems [11, 12], to solve optimization problems in var-

ious technical systems [13–15].

One of the areas of research in the field of genetic algorithms involves their use in combination with other methods (penalty method [16]; method based on the calculation of covariance matrices [17]). However, the use of third-party methods leads to the need to select the values of additional parameters. This entails the need to study the influence of the values of additional parameters on the results obtained. Another area is associated with modifications of the operations of selection, crossing, mutation depending on the specifics of the problem being solved. In this case, no additional parameters or transformations of the original problem are required.

The paper [18] presents an algorithm for calculating the optimal initial concentrations of substances in chemical reactions based on the heuristic method of artificial immune systems, which has been tested on the industrially significant process of synthesizing benzylidene benzylamine. The disadvantage of this algorithm is the lack of a stage for checking the condition of equality of the sum of the calculated initial concentrations to a given value (for example, one if the concentration is expressed in mole fractions). Therefore, the algorithm can be used for reactions that contain two starting substances. However, complex chemical transformations often occur with the participation of three or more starting substances.

The aim of the work is to develop a genetic algorithm for solving the problem of determining the optimal initial concentrations of a complex chemical reaction.

2 Materials and methods

Let the dynamics of concentrations of substances of a complex chemical reaction over a period of time $[0, \tau]$ be described by a system of ordinary differential equations

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

with initial conditions

$$x_i(0) = x_i^0, \quad i = \overline{1,n}, \tag{2}$$

where $x(t) = (x_1(t), x_2(t), ..., x_n(t))^T$ – vector of substance concentrations, t – time, T – temperature, $f(t, x(t), T) = (f_1(t, x(t), T), \ldots, f_n(t, x(t), T))^T$ – vector function continuous together with its partial derivatives.

Let values of concentrations of substances are expressed in mole fractions. Then at the initial moment of time the following relation is fulfilled:

$$\sum_{i=1}^{n} x_i^0 = 1. \tag{3}$$

There are restrictions on the values of the initial concentrations of substances:

$$0 \le x_i^0 \le 1, \quad i = \overline{1,n}. \tag{4}$$

Consider the problem of optimizing a function of the form

$$J(x^0) = \varphi(x(\tau)). \tag{5}$$

Then the problem of optimizing the initial concentrations of a chemical reaction consists of finding the vector $x^0 = (x_1^0, ..., x_n^0)$ taking into account conditions (3), (4), under which the functional (5) reaches its maximum value.

Let us formulate a genetic algorithm with real coding for solving this problem. The work of the genetic algorithm consists of changing generations of vectors-individuals, which represent possible solutions to the optimization problem (1)–(5). The set of vectors-individuals forms a population [19]. Therefore, we will consider a set of m vectors as a population:

$$x_j^0 = (x_{j1}^0, x_{j2}^0, ..., x_{jn}^0), \quad j = \overline{1,m}, \tag{6}$$

where x_j^0 is the j-th individual. The elements of the vector x_j^0 are the genes on which the crossover and mutation operations are performed. The quality of each individual (possible solution) is determined by the value of

the fitness function. The fitness function is function (5) in the optimization problem (1)–(5). The fittest individual corresponds to the highest value of the fitness function, since the problem is solved for the maximum. In order to calculate the value of the fitness function, it is necessary to find a numerical solution to the system of differential equations (1) with the initial conditions (2).

The optimization problem (1)–(5) has a number of features associated with its physical and chemical meaning.

Firstly, it is necessary to provide for the fulfillment of conditions (3), (4) at the stage of generating the initial population. Secondly, it is necessary to control the fulfillment of condition (3) at the stages of crossing and mutation, since it can be violated. This can be done by normalizing the coordinates of the individual vector. Therefore, it is necessary to make an adjustment to the values of the components of vectors (6) in the genetic algorithm, taking into account conditions (3), (4).

Let us modify the genetic algorithm to solve the problem of searching for optimal initial concentrations of chemical reaction substances.

Step 1. Set the algorithm parameters: population size m, algorithm termination parameters q, $\varepsilon > 0$. Set the population counter $k = 0$.

Step 2. Generate the initial population $x_j^0(0)$. Fill the components of individuals with random values from the region defined by inequality (4).

Check the condition of equality of the total concentration of substances to one (condition (3)) for each vector $x_j^0(0)$, $j = \overline{1,m}$. If $\sum\limits_{l=1}^{n} x_{jl}^0(0) = 1$, then go to step 3. Otherwise, recalculate the components of the vector $x_j^0(0)$ so that they add up to one.

Step 3. Calculate the value of the fitness function (5) for each vector of initial concentrations $x_j^0(k)$ $(j = \overline{1,m})$ of the current k-th population.

Step 4. Apply the selection operator "panmixia", which consists of random equiprobability selection of a parental pair. Randomly select two initial concentration vectors $x_l^0(k)$, $x_s^0(k)$. The parental pair $y^1 = x_l^0(k)$, $y^2 = x_s^0(k)$ is the result of step 4.

Step 5. Apply linear crossover to the vectors y^1, y^2, selected in step 4.

Create three child vectors r^1, r^2, r^3:

$$r_i^1 = \frac{y_i^1 + y_i^2}{2}, \quad r_i^2 = \frac{3y_i^1 - y_i^2}{2}, \quad r_i^3 = \frac{y_i^2 - 3y_i^1}{2}, \quad i = \overline{1,n}.$$

Step 6. Check the fulfillment of condition (4) for the descendant vectors r^s $(s = 1, 2, 3)$. If $r_i^s < 0$ or $r_i^s > 1$ $(s = 1, 2, 3)$, then replace r_i^s with a random value from the range $[0, 1]$.

Step 7. Check the fulfillment of condition (3) for each of the vectors r^s $(s = 1, 2, 3)$. If it is not fulfilled, then transform the coordinates of the vector r^s:

$$r_i^s = \frac{r_i^s}{\sum\limits_{l=1}^{n} r_l^s}, \quad i = \overline{1,n}. \tag{7}$$

Step 8. Create mutant vectors from descendant vectors r^1, r^2, r^3 by applying the random mutation operator. Randomly select the r_l^s gene for each of the r^s $(s = 1, 2, 3)$ vectors. Replace the r_l^s gene value with a random number from the interval specified by inequality (4). As a result of applying the mutation operator, the sum of the values of the components of the r^s vector may differ from 1, i.e. condition (3) is violated. In this case, it is necessary to transform the coordinates of the r^s vector using formula (7).

Step 9. Update the current population. Among the initial concentration vectors, find the vector for which function (5) takes the smallest value. Replace this vector with a randomly selected mutant vector. Calculate the fitness function value for it. Increase the population counter k by 1 and go to step 10.

Step 10. Check the condition for ending the search for a solution. Calculate the distance between the vectors of the current $x_i^0(k)$ and the previous $x_j^0(k-1)$ populations $(i, j = \overline{1,m})$. If the condition $\|x_i^0(k) - x_j^0(k-1)\| < \varepsilon$ is met over q generations, i.e. there is an insignificant change in the population, then stop searching for a solution. From the last population, find the vector of initial concentrations x_j^0 that corresponds to the highest value of the fitness function. The selected vector x_j^0 is an approximate solution to the problem of determining the optimal initial concentrations of a chemical reaction. Otherwise, go to step 4.

The developed algorithm takes into account a number of features related to the physicochemical meaning of the problem (1)–(5):

1) at the stage of formation of the initial population, the recalculation of the values of the initial concentrations is provided in case of violation of condition (3) (step 2);

2) at the crossover stage, the fulfillment of condition (3) is checked for the descendant individuals (step 6) and the values of their components are recalculated in case of violation of the condition of equality of the total concentration to one (step 7);

3) at the mutation stage, the condition of the values of the mutant vector components going beyond the limits of the permissible range is checked (step 8).

3 Research results

Let us calculate the optimal initial concentrations of reagents for the reaction of benzyl butyl ether synthesis under the action of copper-containing catalysts using the developed algorithm. The mechanism of this reaction is described by the following stages of chemical transformations [20]:

$$\begin{gathered} X_1 + X_2 \to X_3, \\ X_3 + X_4 \to X_5, \\ X_5 \to X_6 + X_7 + X_2, \\ X_3 + X_1 \to X_8, \\ X_8 \to X_9 + X_7 + X_2, \\ X_2 + X_4 \to X_{10}, \\ X_{10} + X_4 \to X_{11}, \\ X_{11} \to X_{12} + X_7 + X_2, \\ X_{10} + X_1 \to X_5, \end{gathered} \tag{8}$$

where X_1 is $PhCH_2OH$, X_2 is $CuBr_2$, X_3 is $[PhCH_2]^+[CuBr_2(OH)]^-$, X_4 is BuOH, X_5 is $[PhCH_2OBu]H^+[CuBr_2(OH)]^-$, X_6 is $PhCH_2OBu$, X_7 is H_2O, X_8 is $[PhCH_2OHCH_2Ph]^+[CuBr_2(OH)]^-$, X_9 is $PhCH_2OCH_2Ph$, X_{10} is $[Bu]^+[CuBr_2(OH)]^-$, X_{11} is $[BuOHBu]^+[CuBr_2(OH)]^-$, X_{12} is

BuOBu.

According to the law of acting masses, the equations of rates of reaction stages have the form:

$$\begin{aligned} w_1(C,T) &= k_1(T)C_1C_2, \\ w_2(C,T) &= k_2(T)C_3C_4, \\ w_3(C,T) &= k_3(T)C_5, \\ w_4(C,T) &= k_4(T)C_1C_3, \\ w_5(C,T) &= k_5(T)C_8, \\ w_6(C,T) &= k_6(T)C_2C_4, \\ w_7(C,T) &= k_7(T)C_1C_4, \\ w_8(C,T) &= k_8(T)C_{11}, \\ w_9(C,T) &= k_9(T)C_1C_{10}, \end{aligned} \tag{9}$$

where C_i is the concentration of substance X_i (mol/l, $i = \overline{1,12}$), T is the temperature (K), $k_j(T)$ is the kinetic constant (l/(mol·min), $j = 1,2,4,6,7,9$; 1/min, $j = 3,5,8$), calculated by the Arrhenius equation

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

where k_{0j} is the pre-exponential multiplier (l/(mol·min), $j = 1,2,4,6,7,9$; 1/min, $j = 3,5,8$), E_j is the activation energy of the j-th stage (kJ/mol), R is the universal gas constant (8,31 J/(mol·K)). The values of the rate constants k_j and the activation energies E_j ($j = \overline{1,9}$) of the stages of the benzyl butyl ether synthesis reaction are given in [20].

Let $x_i = C_i/C_0$ – concentration of substance X_i expressed in mole fractions, C_0 – initial total concentration of substances (mol/l). Then the change of concentration of substances of reaction (8) in time is described

by a system of ordinary differential equations:

$$\begin{aligned}
\frac{dx_1}{dt} &= -w_1 - w_4 - w_9,\\
\frac{dx_2}{dt} &= -w_1 + w_3 + w_5 - w_6 + w_8,\\
\frac{dx_3}{dt} &= w_1 - w_2 - w_4,\\
\frac{dx_4}{dt} &= -w_2 - w_6 - w_7,\\
\frac{dx_5}{dt} &= w_2 - w_3 + w_9,\\
\frac{dx_6}{dt} &= w_3,\\
\frac{dx_7}{dt} &= w_3 + w_5 + w_8,\\
\frac{dx_8}{dt} &= w_4 - w_5,\\
\frac{dx_9}{dt} &= w_5,\\
\frac{dx_{10}}{dt} &= w_6 - w_7 - w_9,\\
\frac{dx_{11}}{dt} &= w_7 - w_8,\\
\frac{dx_{12}}{dt} &= w_8,
\end{aligned} \tag{10}$$

with initial conditions

$$x_i(0) = x_i^0, \quad i = \overline{1,12}, \tag{11}$$

where $x(t) = (x_1(t), ..., x_{12}(t))^T$ is the vector of substance concentrations (mole fraction), $t \in [0, \tau]$ is time.

The initial substances of reaction (8) are X_1, X_2, X_4. The values of the initial concentrations of these substances must satisfy the conditions:

$$0 < x_i^0 < 1, \quad i = 1, 2, 4, \tag{12}$$

$$x_1^0 + x_2^0 + x_4^0 = 1. \tag{13}$$

The concentration values of the other substances are zero: $x_i^0 = 0$, $i = \overline{3, 5, 12}$.

The products of reaction (8) are benzyl butyl ether X_6 and dibenzyl ether X_9, which are widely used as flavouring agents in perfumery and cosmetic industries.

We will search for the maximum concentration value of the target sub-

stances at the end of the reaction ($t = \tau$):

$$J(x^0) = x_6(\tau) + x_9(\tau) \to \max. \tag{14}$$

It is required to determine the initial concentrations of initial substances x_1^0, x_2^0, x_4^0, at which function (14) reaches the highest value.

To solve the problem (8)–(14), a program in the Delphi language has been developed, in which the algorithm developed by the authors is implemented. The solution to the problem has been found for a reaction with a duration of $\tau = 480$ min with the following algorithm parameters: population size $m = 60$, algorithm termination parameters $q = 5$, $\varepsilon = 10^{-3}$. The calculations are performed for temperature $T = 433$ K.

The second-order Adams predictor-corrector method is applied for numerical solution of the system of differential equations (10) with initial conditions (11).

As a result of the calculations, the following values of the initial concentrations of the reagents (mole fraction) have been calculated:

$$x_1^0 = 0,42, \quad x_2^0 = 0,28, \quad x_4^0 = 0,3. \tag{15}$$

The highest value of the concentration of the target reaction products is 0,278 mole fractions.

Fig. 1, 2 shows the dynamics of the concentrations of initial substances and target products of reaction (8), calculated with a set of initial concentrations (15). Fig. 1 shows that the concentration of target reaction products X_6, X_9 increases monotonically throughout the entire reaction time.

The concentration of reagent X_1, shown in Fig. 2, decreases monotonically with time. This is due to the consumption of the substance in the first, fourth and ninth stages.

Reagent X_4 is consumed in the second, sixth and seventh stages of the reaction. Therefore, the dependence of its concentration on time is a monotonically decreasing function (Fig. 2).

Substance X_2 is consumed in the first and sixth stages. Therefore, its concentration decreases until the time $t \approx 50$ min. Then, until the

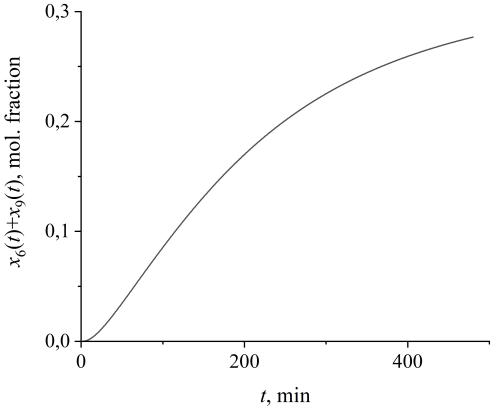

Figure 1. Dynamics of concentrations of substances X_6, X_9

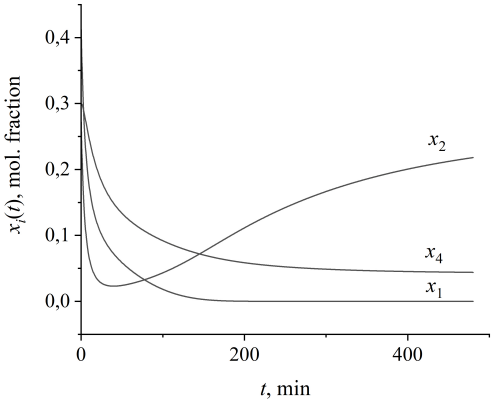

Figure 2. Dynamics of concentrations of substances X_1, X_2, X_4

end of the reaction, the concentration of X_2 increases. This is due to the predominance of its synthesis in the third, fifth, eighth stages over consumption (Fig. 2).

The numerical solution of the system of differential equations (10) with different sets of initial conditions (11) also has been found (Table 1). The

table shows that the calculated concentration values of the target reaction products at the final moment of time do not exceed the value found for the initial concentrations (15).

Table 1. Values of concentrations of target substances calculated at different initial concentrations of initial substances

No.	x_1^0, mol. fraction	x_2^0, mol. fraction	x_4^0, mol. fraction	$x_6(\tau) + x_9(\tau)$, mol.fraction
1	0,7	0,1	0,2	0,109
2	0,6	0,1	0,3	0,135
3	0,45	0,1	0,45	0,176
4	0,3	0,1	0,6	0,200
5	0,2	0,1	0,7	0,163
6	0,4	0,2	0,4	0,269
7	0,3	0,2	0,5	0,234
8	0,5	0,2	0,3	0,266
9	0,5	0,25	0,25	0,267
10	0,25	0,25	0,5	0,209
11	0,5	0,3	0,2	0,246
12	0,4	0,3	0,3	0,275
13	0,35	0,3	0,35	0,265
14	0,3	0,3	0,4	0,242
15	0,2	0,3	0,5	0,176

Let us compare the calculated solution of problem (8)–(14) with the solution obtained using the Hook-Jeeves method. We will apply the penalty method to control the fulfillment of conditions (12), (13).

The authors have developed a program in Delphi for solving problem (8)–(14) based on the penalty and Hook-Jeeves methods. The following parameters are applied: initial penalty value – 1, penalty increase parameter – 8, initial vector of reagent concentrations (mole fraction) – $x^0 = (0,45; 0,1; 0,45)$, step in coordinate directions – 0,1, accelerating factor – 0,3, step decrease parameter – 2.

The following solution to problem (8)–(14) (mole fraction) is obtained:

$$x_1^0 = 0,41, \quad x_2^0 = 0,29, \quad x_4^0 = 0,3.$$

The highest concentration of target products at the end of the reaction is 0,277 mole fractions. The relative errors of the values of the initial concentrations of the reagents and the concentration of the target reaction products are calculated: $\delta(x_1^0) = 2,4\%$, $\delta(x_2^0) = 3,4\%$, $\delta(x_4^0) = 0$, $\delta(J(x^0)) = 0,36\%$. From this it is clear that the solution to problem (8)–(14), found using the genetic algorithm, differs slightly from the solution calculated using the penalty and Hook-Jeeves methods. Therefore, we can conclude that the developed algorithm for determining the optimal concentrations of chemical reaction reagents works correctly.

4 Conclusion

The developed genetic algorithm allows finding an approximate solution to the problem of determining the optimal initial concentrations of a chemical reaction. The vector of initial concentrations of reagents is considered as an individual vector. Modifications have been made to the classical genetic algorithm with real coding taking into account the physicochemical meaning of the problem. The changes concern the stages of filling the initial population, crossover and mutation. If the sum of the values of the components of the initial concentration vector exceeds one or goes beyond the boundaries of the range of acceptable values, then the coordinates of the individual vector are transformed.

The work of the genetic algorithm has been tested on the reaction of benzyl butyl ether synthesis. The mathematical description of this catalytic reaction is a system of nonlinear differential equations. The initial concentrations of the reagents at which the highest values of the concentrations of the reaction products – benzyl butyl ether and dibenzyl ether – are achieved have been determined.

The developed genetic algorithm is easy to implement in practice. It can be used to calculate the optimal values of reagent concentrations for a reaction involving three or more initial substances.

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References

[1] D. Mu, C. Xu, Z. Liu, Y. Pang, Further insight into bifurcation and hybrid control tactics of a chlorine dioxide-iodine-malonic acid chemical reaction model incorporating delays, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 529–566.

[2] F. A. Shatkhan, Application of the maximum principle to problems of optimization of parallel chemical reactions, *Autom. Remote Control* **3** (1964) 368–373. (in Russ.)

[3] A. I. Baitimerova, S. A. Mustafina, S. I. Spivak, Optimization of catalytic reaction of dimerization of α-methylstyrene on the basis of kinetic model, *Bashkir Chem. J.* **2** (2008) 86–88. (in Russ.)

[4] S. A. Dadebo, K. B. Mcauley, Dynamic optimization of constrained chemical engineering problems using dynamic programming, *Comput. Chem. Eng.* **19** (1995) 513–525.

[5] S. Katoch, S. S. Chauhan, V. A. Kumar, A review on genetic algorithm: past, present, and future, *Multimed. Tools Appl.* **80** (2021) 8091–8126.

[6] E. V. Antipina, A. F. Antipin, S. A. Mustafina, Search for the optimal regime parameters of a catalytic process based on evolutionary computations, *Theor. Found. Chem. Eng.* **56** (2022) 162–169.

[7] A. Wright, Genetic algorithms for real parameter optimization, *Found. Genet. Algor.* **1** (1991) 205–218.

[8] X. C. Zhao, X. S. Gao, Z. C. Hu, Evolutionary programming based on non-uniform mutation, *Appl. Math. Comput.* **192** (2007) 1–11.

[9] D. J. Kozuch, F. H. Stillinger, P. G. Debenedetti, Genetic algorithm approach for the optimization of protein antifreeze activity using molecular simulations, *J. Chem. Theory Comput.* **16** (2020) 7866–7873.

[10] E. V. Antipina, S. I. Mustafina, A. F. Antipin, S. A. Mustafina, Algorithm for solving a multiobjective optimization problem on the basis of a kinetic chemical reaction model, *Optoel. Instrum. Proc.* **57** (2021) 124–131.

[11] J. Stastny, V. Skorpil, Z. Balogh, R. Klein, Job shop scheduling problem optimization by means of graph-based algorithm, *Appl. Sci.* **11** (2021) #1921.

[12] R. Gulbaz, A. B. Siddiqui, N. Anjum, Balancer genetic algorithm-a novel task scheduling optimization approach in cloud computing, *Appl. Sci.* **11** (2021) #6244.

[13] Z. Jalali, E. Noorzai, S. Heidari, Design and optimization of form and facade of an office building using the genetic algorithm, *Sci. Technol. Built Environ.* **26** (2020) 128–140.

[14] L. Xie, Y. Chen, R. Chang, Scheduling optimization of prefabricated construction projects by genetic algorithm, *Appl. Sci.* **11** (2021) #5531.

[15] D. A. Migov, K. A. Volzhankina, A. S. Rodionov, Genetic algorithms for drain placement in wireless sensor networks optimal by the relibility criterion, *Optoel. Instrum. Proc.* **57** (2021) 240–249.

[16] E. V. Antipina, S. A. Mustafina, A. F. Antipin, Algorithm for finding an approximate solution of the problem of optimal control of a chemical process in the presence of terminal restrictions, *Tomsk State Univ. J. Control Comput. Sci.* **59** (2022) 4–12. (in Russ.)

[17] D. Ovsyannikov, L. Vladimirova, I. Rubtsova, A. Rubanik, V. Ponomarev, Modified genetic algorithm of global extremum search in combination with directional methods, *Bull. Irkutsk State Univ. Ser. Math.* **39** (2022) 17–33. (in Russ.)

[18] E. V. Antipina, A. F. Antipin, Algorithm for calculation of optimal initial concentrations of chemical reactions substances, *Her. Technol. Univ.* **13** (2017) 84–87. (in Russ.)

[19] A. P. Karpenko, *Modern Search Engine Optimization Algorithms. Algorithms Inspired by Nature*, MSTU im. N. E. Bauman, Moscow, 2014. (in Russ.)

[20] K. F. Koledina, I. M. Gubaidullin, S. N. Koledin, A. R. Baiguzina, L. I. Gallyamova, R. I. Khusnutdinov, Kinetics and mechanism of the syntesis of benzylbutil ether in the presence of copper-containing catalysts, *Russ. J. Phys. Chem.* **93** (2019) 2146–2151.