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Application of a genetic algorithm for optimization of periodic polymerization processes

Aplicación de un algoritmo genético para la optimización de procesos de polimerización periódica

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Abstract
A numerical algorithm for optimal composition search of the initial reaction mixture using heuristic optimization methods is developed and evaluated for its effectiveness in investigating polymer synthesis processes. The methodology, based on a kinetic approach grounded in the method of moments, presents all main stages of the research. A genetic algorithm is proposed for solving the optimization problem of the formed unified model description of the process, with its implementation steps contributing to finding the global optimum. The software implementation of this algorithm and the computational experiments conducted for the production process of 1,4-cis-polyisoprene in the presence of a catalytic system based on neodymium chloride solvates allowed the identification of the initial reaction mixture composition, which contributes to achieving a final conversion of 72% over 85 minutes for a polymer product with a weight-average molecular weight of $680{\cdot}10^3$ g/mol. The proposed algorithm successfully copes with multi-factor optimization tasks.
Keywords: genetic algorithm, optimization, polymerization, heuristic method.

Resumen
Se ha desarrollado un algoritmo numérico para la búsqueda de la composición óptima de la mezcla de reacción inicial mediante métodos de optimización heurística y se ha evaluado su eficacia en la investigación de los procesos de síntesis de polímeros. La metodología, basada en un enfoque cinético apoyado en el método de momentos, presenta todas las etapas principales de la investigación. Se propone un algoritmo genético para resolver el problema de optimización de la descripción del modelo unificado formado del proceso, con sus pasos de implementación que contribuyen a encontrar el óptimo global. La implementación informática de este algoritmo y los experimentos computacionales realizados para el proceso de obtención de 1,4-cis-poliisopreno en presencia de un sistema catalítico basado en solvatos de cloruro de neodimio permitieron identificar la composición inicial de la mezcla de reacción, lo que contribuye a alcanzar en 85 minutos de proceso una conversión final del 72% para un producto polimérico con una masa molecular promedio en peso de $680{\cdot}10^3$ g/mol. El algoritmo propuesto afronta con éxito las tareas de optimización multifactorial.
Palabras clave: algoritmo genético, optimización, polimerización, método heurístico.

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1 Introduction

Polymer synthesis processes play a pivotal role in contemporary chemical industry, as the resultant end products find wide application across diverse scientific and engineering realms. These processes are characterized by sufficiently intricate dynamics, demanding meticulous planning and control at every stage of production. Due to the complex nature of polymer structures and their molecular weight distribution heterogeneity, the evaluation of physicochemical parameters typically relies on the utilization of averaged molecular characteristics (Greene, 2001; Yigit *et al*., 2019; Gao and Penlidis, 2002; Pereira and Giudici, 2023), the numerical representation of which is influenced by both the composition of the utilized reaction mixture and the technological parameters of continuous production (Hamielec *et al*., 1987; Luciani and Choi, 2021; Rawlings and Ekerdt, 2002; Aris, 1989; Zamora Cisneros and Ruiz Martínez, 2023).

Despite extensive historical experience, enterprises are compelled to constantly respond to modern requirements for the resultant polymer product and adjust the fundamental technological stages of production. In the context of production modernization, addressing the challenge of obtaining a product with specified structure and properties remains highly relevant today, necessitating iterative exploration of optimal conditions through the organization of numerous empirical investigations. It is evident that conducting such research within the confines of existing laboratory/industrial production conditions is practically infeasible, thus highlighting the increasing relevance of a mathematical approach, which, through model description of the process and organization of a series of computational experiments, enables the assessment of fundamental process trends and determination of optimal conditions.

The mathematical description of a complex physicochemical process entails accounting for all significant production factors influencing the rate of progression and properties of the resulting product. The high dimensionality and nonlinear nature of the mathematical description dictate the necessity of employing nontrivial approaches and methods capable of finding a global solution within a short timeframe.

In the context of solving optimization problems in complex processes, heuristic optimization methods (Almufti *et al*., 2023; Panteleev *et al*., 2024; Simon, 2013) are particularly attractive, as they provide necessary tools for the analysis and enhancement of reaction mechanisms, kinetic parameters, and reaction conditions. In conjunction with modern computational technologies, heuristic methods open up new avenues for understanding and controlling chemical processes and systems. The utilization of heuristic methods for addressing the task of identifying optimal modes of polymer production holds significant scientific and practical interest.

The objective of this work is to develop a numerical algorithm for solving the problem of finding the optimal composition of the initial reaction mixture using heuristic optimization methods, and to evaluate its effectiveness in studying periodic polymerization processes.

2 Materials and methods

All optimization problem-solving algorithms are based on a formalized description of the process, which constitutes the primary mathematical model. This model encompasses both the fundamental equations describing the material balance changes for each reaction component and additional parameters influencing the process. It is evident that the modeling representation often varies depending on the conditions of the process, the scale of description, and the mathematical approach employed.

To standardize the methodology and algorithm for solving optimization problems, let us outline the main stages of modeling in the form of a unified comprehensive approach to investigating polymer synthesis processes.

Stage 1 involves conducting a series of laboratory experiments to identify primary physicochemical information in the form of data on polymerization rate and molecular weight distribution (MWD) of the resultant product. The experimental results are essential for assessing kinetic heterogeneity (Miftakhov *et al*., 2021, 2022), refining the kinetic mechanism of elementary reactions, as well as formulating and solving inverse problems to identify some of the unknown kinetic parameters.

Further research is impossible without knowledge of the quantity and proportion of active centers (Piña-Victoria *et al*., 2024) initiating the polymerization process. To assess kinetic heterogeneity, it is necessary to represent the initial MWD curve as a superposition of distributions (Usmanov *et al*., 2005) formed by each active center and estimate the corresponding proportions of each. Figure 1 illustrates an example of such decomposition for a titanium-containing catalytic system used in the production of 1,4-cis-polyisoprene (Miftakhov *et al*., 2023). Analysis of the obtained decomposition, conducted earlier in the study (Zakharov *et al*., 2015), led to the conclusion that this type of catalyst exhibits the presence of 2 types of active centers.

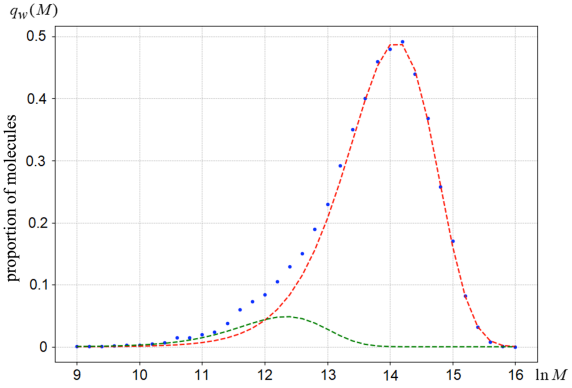


Figure 1. The results of the investigation into the kinetic heterogeneity of 1,4-cis-polyisoprene (*points* represent the original MWD curve, and the dashed lines represent the calculated curves for active centers of types 1 and 2, M – molecular weight).

To address the tasks related to the investigation of kinetic heterogeneity, both the Tikhonov regularization method (Tikhonov and Arsenin, 1986; Albani *et al*., 2016), extensively discussed in previous Works (Zakharov *et al*., 2015; Miftakhov *et al*., 2022), and an original simulation-based approach (Miftakhov *et al*., 2024) to solving inverse problems are utilized.

Stage 2 involves describing the kinetic mechanism of the process, which includes the primary elementary reactions leading to the formation of high-molecular-weight compounds. It is evident that in conditions of mono- and polycentered catalyst nature, the formulation of the kinetic mechanism varies and depends on the results obtained from the first stage of modeling. The kinetic mechanism under conditions of monocentered catalyst nature encompasses stages

1. Chain growth of the polymer

$$P_i + M \xrightarrow{k_p} P_{i+1},$$

2. Chain transfer to a monomer molecule

$$P_i + M \xrightarrow{k_m} Q_i + P_1,$$

3. Chain transfer to a regulator (aluminum-organic compound)

$$P_i + A \xrightarrow{k_a} Q_i + P_1,$$

4. Possible deactivation of active centers

$$P_i \xrightarrow{k_d} Q_i,$$

where M represents the monomer, A – denotes the regulator (aluminum-organic compound), P_i – signifies an active («growing») polymer chain of length i; Q_i – represents an inactive («dead») polymer chain of length i, k_p, k_m, k_a, k_d – kinetic parameters characterizing the rates of individual elementary reactions.

In conditions of a polycentered catalyst nature, it is necessary to identify active polymer chains P_i^j with an additional parameter j, characterizing the type of active center at the end of the growing macromolecule, $j = 1..n$ (n – represents the number of different active centers). The kinetic mechanism should also include the potential mutual transfer of active centers.

Stage 3 involves employing a kinetic approach to mathematically describe the periodic polymerization process. The kinetic approach is based on representing the main mechanism of the process as a system of ordinary differential equations characterizing the material balance changes for each reaction component and numerically solving it.

For the kinetic scheme presented above, the system of differential equations takes the form

$$\begin{cases} \frac{dM}{dt} = -M\sum_{i=0}^{\infty} P_i\left(k_p + k_m\right), \\ \frac{dA}{dt} = -k_a A\sum_{i=0}^{\infty} P_i, \\ \frac{dP_1}{dt} = -k_p M P_1 + (k_m M + k_a A)\sum_{i=2}^{\infty} P_i, \\ \frac{dQ_1}{dt} = k_m M P_1 + k_a A P_1, \\ \frac{dP_i}{dt} = k_p M(P_{i-1} - P_i) - k_m M P_i - k_a A P_i - k_d P_i, \\ \frac{dQ_i}{dt} = k_m M P_i + k_a A P_i + k_d P_i. \end{cases} \quad (1)$$

where $A(0) = A_0, M(0) = M_0, P_i(0) = Q_i(0) = 0$ for any i. Due to the sufficiently high dimensionality of the system (1), a transition to averaged molecular characteristics is employed using statistical moments of the molecular weight distribution

$$\mu_j = \sum_{i=2}^{+\infty} i^j P_i, \eta_j = \sum_{i=2}^{+\infty} i^j Q_i \quad (2)$$

In this case, the system of differential equations describing the process takes the form

$$\begin{cases} \frac{dM}{dt} = -MP_1\left(k_p + k_m\right) - M\mu_0\left(k_p + k_m\right), \\ \frac{dA}{dt} = -k_a A P_1 - k_a A\mu_0, \\ \frac{dP_1}{dt} = -k_p M P_1 + (k_m M + k_a A)\mu_0, \\ \frac{dQ_1}{dt} = k_m M P_1 + k_a A P_1, \\ \frac{d\mu_0}{dt} = k_p M P_1 - (k_m M + k_a A + k_d)\mu_0, \\ \frac{d\eta_0}{dt} = (k_m M + k_a A + k_d)\mu_0, \\ \frac{d\mu_1}{dt} = 2k_p M P_1 + k_p M\mu_0 - (k_m M + k_a A + k_d)\mu_1, \\ \& \frac{d\eta_1}{dt} = (k_m M + k_a A + k_d)\mu_1, \\ \frac{d\mu_2}{dt} = 4k_p M P_1 + k_p M\mu_0 + 2k_p M\mu_1 - (k_m M + k_a A + k_d)\mu_2, \\ \frac{d\eta_2}{dt} = (k_m M + k_a A + k_d)\mu_2, \end{cases} \quad (3)$$

where $M(0) = M_0$, $A(0) = A_0$, $P_1(0) = P_0$, $Q(0) = 0$, $\mu_i(0)=\eta_i(0)=0$, $i = 0..2$.

Stage 4. Numerical solution of the obtained system of differential equations. This stage involves using explicit and implicit schemes for organizing numerical calculations to obtain dependencies of changes in the concentrations of the starting reagents and moments of the molecular weight distribution over time.

For calculating averaged molecular characteristics, represented by the number-average molecular weight ($\overline{M_n}$) and the weight-average molecular weight ($\overline{M_w}$), knowledge of initial moments is required:

$$\overline{M}_n = m_0 \frac{\mu_1 + \eta_1}{\mu_0 + \eta_0}, \overline{M}_w = m_0 \frac{\mu_2 + \eta_2}{\mu_1 + \eta_1}, \quad (4)$$

where m_0 – molar mass of monomer.

Stage 5. Evaluation of the obtained results and comparative analysis with data from conducted laboratory experiments. The conducted analysis allows for refining the formulation of the kinetic mechanism of elementary reactions and the values of kinetic parameters characterizing the rates of individual elementary stages.

Previously, in the work (Miftakhov *et al*., 2021), such an approach allowed for the reconstruction of the formulation of the kinetic mechanism for the process of obtaining 1,4-cis-polyisoprene. It is evident that stages 1-5 can be conducted iteratively until obtaining results that consistently reflect experimental outcomes under various initial conditions.

Stage 6. Formulation and solving of the optimization problem. In the context of periodic process operation, this stage entails determining the optimal composition of the initial reaction mixture that facilitates the production of a product with the desired structure and properties (Guzman-Lucero *et al*., 2024).

Within the framework of implementing the kinetic approach, the mathematical model of the process constitutes a system of ordinary differential equations of the form

$$\frac{dX_i}{dt} = F_i(t, X_i(t)), i = 1 \ldots n \quad (5)$$

with initial conditions $X_i(0) = X_i^0$ for any $i = 1..n$, where $X(t)$ – vector that determines the concentrations of all initial components of the reaction at a point in time $t \in [0, t_{end}]$.

If $\widetilde{X}$ characterizes a certain output state of the system, then within the framework of implementing this stage, it is necessary to determine the vector of initial concentrations of the starting components of the system $X^*(0) = (x_1^*(0), x_2^*(0), ..., x_n^*(0))$, at which, at the final moment of simulation t_{end} the system will transition to the desired state $\widetilde{X}$.

It is evident that $\widetilde{X}$ can reflect the state of the system across multiple parameters simultaneously. In this case, as a criterion of optimality, one can consider a functional of the form

$$G(X^*(0)) = \sum_{i=1}^{m} \left(X_i(t_{end}) - \widetilde{X}_i \right) \to min, m \le n, \quad (6)$$

where m – number of system states being studied.

In the context of solving control problems for such complex physicochemical processes, preference is given to optimization methods that guarantee finding the global optimum of the problem. Heuristic optimization methods demonstrate themselves most vividly in this area, among which genetic algorithms (Simon, 2013; Katoch *et al*., 2021; Kasat *et al*., 2003; Kim *et al*., 2021) hold a leading position, based on the mechanism of creating a population of potential solutions using probabilistic laws (Holland, 1992). To implement a genetic algorithm, iterative execution of the following steps is required:

Step 1. An initial population of possible solutions is defined for each component of the system

$$X = x_{ij}(0) = \underline{x_i} + \frac{\overline{x_i} - \underline{x_i}}{(K-1)} \cdot (j-1), j = 1 \ldots K, \quad (7)$$

where $\underline{x_i}$, $\overline{x_i}$ are the lower and upper boundaries of the segment that defines the restriction for x_i.

Step 2. For each proposed solution, the degree of adaptability is evaluated by calculating the value of the objective function $G(X_j), j = 1..K$. Based on the obtained values, the probability of selecting each solution for participation in the subsequent population is determined. Solutions demonstrating more optimal values of the objective function are more likely to be included in the pool for offspring creation.

Step 3. From the created parental pool, the procedure of obtaining K offspring is conducted using the crossover operator. For two parental individuals of the form $X^1 = (x_1^1, x_2^1, ..., x_n^1)$ and $X^2 = (x_1^2, x_2^2, ..., x_n^2)$, in the case of using arithmetic crossover, the values of the offspring vector are formed according to the rule:

$$y_i = a \cdot x_i^1 + (1-a) \cdot x_i^2, i = 1 \ldots n, \quad (8)$$

where a is the coefficient of the operator from the interval (0, 1).

Step 4 involves assessing the fitness of each individual in the new population. If the value of the objective function meets the criterion $G(X_j) \le \varepsilon, j = 1..K$, the algorithm should be stopped, and the solution found should be outputted. Otherwise, steps 2-4 are repeated for further reproduction and obtaining more fit offspring.

To prevent the algorithm from converging to a local extremum due to premature population "degeneration," an additional step is taken to perform the mutation operator. The main goal of this step is to introduce genetic diversity into the population. For this purpose, a parameter p_m is introduced to determine the probability of randomly changing elements in the vector of offspring. The elements in the vector undergoing mutation are altered according to the rule $x_i = x_i \pm \alpha \cdot \delta$, where δ represents the change in the element within the permissible range and the parameter α serves as a correction coefficient, ranging from 0 to 1.

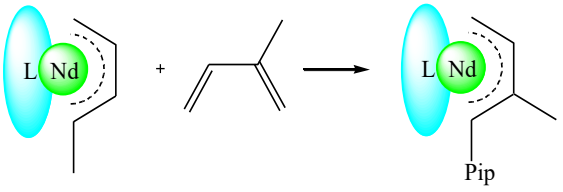
3 Results and discussion

The validation of the genetic algorithm for optimization tasks was conducted for the isoprene polymerization process in the presence of a neodymium-containing catalyst (Zakharov *et al.*, 2013; Tanaka *et al.*, 2016), the composition of which was formulated based on the ratio of $NdCl_3$/triisobutylaluminum (TIBA)/piperylene = 1 mol/12 mol/2 mol. The catalyst dosage was 1 mol per 10^4 mol of isoprene, and the molecular weight was regulated by the addition of diisobutylaluminum hydride (DIBAH). During the catalyst preparation stage, the catalytic complex underwent hydrodynamic treatment using a tubular turbulent apparatus (Berlin *et al.*, 2019; Nasyrov *et al.*, 2021), resulting in the mono-centering of the catalyst.

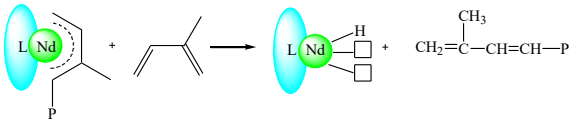
In continuous industrial production, the process line can utilize up to nine cascade reactors with volumes up to 16.6 m^3. All the polymerization reactors used, due to their design features, can be classified as ideal mixing reactors (continuous stirred-tank reactors, CSTRs).

Previous studies have shown that in describing the kinetic mechanism, it is necessary to consider two distinct stages of chain transfer to organoaluminum compounds. The overall kinetic mechanism of such a process is as follows:

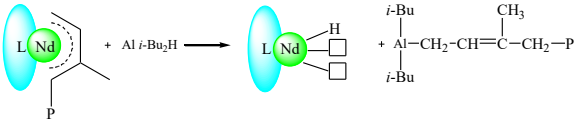
1. Chain propagation



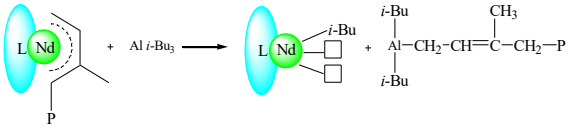
2. Chain transfer to monomer



3. Chain transfer to diisobutylaluminum hydride (DIBAH)



4. Chain transfer to triisobutylaluminum (TIBA)



Using conventional notation for all components of the reaction mixture, the kinetic mechanism can be represented as:

1. Chain propagation $P_i + M \xrightarrow{k_p} P_{i+1}$
2. Chain transfer to monomer $P_i + M \xrightarrow{k_m} Q_i + P_1$
3. Chain transfer to organoluminum compound (TIBA) $P_i + A_{TIBA} \xrightarrow{k_{at}} Q_i + P_1$
4. Chain transfer to organoluminum compound (DIBAH) $P_i + A_{DIBAH} \xrightarrow{k_{ad}} Q_i + P_1$

where M is the monomer concentration; A_{TIBA}, A_{DIBAH} are the concentrations of triisobutylaluminum and diisobutylaluminum hydride, respectively; P_i is an active ("growing") polymer chain of length i, Q_i is an inactive ("dead") polymer chain of length i; k_p, k_m, k_{at}, k_{ad} are the rate constants for chain propagation, chain transfer to monomer, and chain transfer to organoaluminum compounds (TIBA and DIBAH), respectively.

The mathematical model for the presented kinetic mechanism of elementary reactions is represented as:

$$
\begin{cases}
\frac{dM}{dt} = -MP_1\left(k_p + k_m\right) - M\mu_0\left(k_p + k_m\right), \\
\frac{dA_{TIBA}}{dt} = -k_{at}A_{TIBA}P_1 - k_{at}A_{TIBA}\mu_0, \\
\frac{dA_{DIBAH}}{dt} = -k_{ad}A_{DIBAH}P_1 - k_{ad}A_{DIBAH}\mu_0, \\
\frac{dP_1}{dt} = -k_pMP_1 + (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_0, \\
\frac{dQ_1}{dt} = k_mMP_1 + (k_{at}A_{TIBA} + k_{ad}A_{DIBAH})P_1, \\
\frac{d\mu_0}{dt} = k_pMP_1 - (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_0, \\
\frac{d\eta_0}{dt} = (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_0, \\
\frac{d\mu_1}{dt} = 2k_pMP_1 + k_pM\mu_0 - (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_1, \\
\frac{d\eta_1}{dt} = (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_1, \\
\frac{d\mu_2}{dt} = 4k_pMP_1 + k_pM\mu_0 + 2k_pM\mu_1 - (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_2, \\
\frac{d\eta_2}{dt} = (k_mM + k_{at}A_{TIBA} + k_{ad}A_{DIBAH})\mu_2.
\end{cases}
\tag{9}
$$

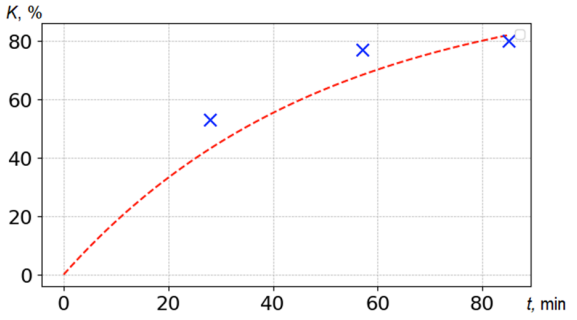


Figure 2. Conversion versus time for the initial composition of the reaction mixture (x – laboratory experiment results; dashed line – calculated results).

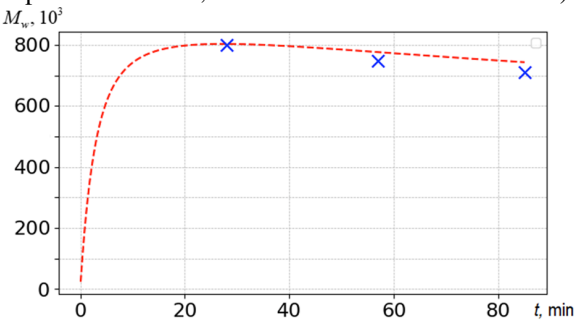


Figure 3. Weight-average molecular weight versus time for the initial composition of the reaction mixture (x – laboratory experiment results; dashed line – calculated results).

Initial conditions for the system (9):

$$M(0)=M_0, A_{TIBA}(0)=A_{TIBA(0)}, A_{DIBAH}(0)=A_{DIBAH(0)},$$
$$P_1(0)=P_0, Q(0)=0, \mu_i(0)=\eta_i(0)=0, i=0\ldots2. \quad (10)$$

For the numerical calculation of the obtained system of differential equations, a custom software implementation of the fourth-order implicit Adams–Moulton method was used. The computational experiments conducted allowed us to obtain the dependencies of conversion and weight-average molecular weight over time (Figures 2 and 3). The points shown on the graphs represent the results of laboratory experiments conducted in the central plant laboratory of the "Sintez Kauchuk" enterprise, which carries out continuous production of this type of product.

The calculated dependencies obtained agree quite well with the results of the laboratory experiments conducted. The root mean square error (RMSE) in calculating the conversion was 7.6%, and in estimating the weight-average molecular weight was $25{\cdot}10^3$. Analysis of the results confirms the adequacy of the presented model of the system and the kinetic parameters used.

We need to determine the initial composition of the reaction mixture that achieves a final conversion $\widetilde{K}$=72% for the polymer product with an average molecular weight $\widetilde{M_w}$=$680{\cdot}10^3$ g/mol in 85 minutes of process operation.

Since the conversion dependency within the specified kinetic mechanism is solely determined by the catalyst concentration, solving the optimization problem of finding the optimal composition of the initial reaction mixture was carried out step by step. This step-by-step approach to solving the optimization problem allowed avoidance of suboptimal solutions when implementing the genetic algorithm, as the individual dependence of the objective function on each of the sought parameters of the system is monotonic. To demonstrate the uniqueness and stability of the found solution, the genetic algorithm was run multiple times with different initial conditions and consistently converged to the same optimal solution. The stages of solving the direct problem for the developed process model and all the steps of the genetic algorithm presented above were programmed in Python (version 3.10.12) and executed in the Google Colab environment.

Stage 1. Identification of the catalyst concentration to achieve the required conversion level. For the implementation of this stage, the minimum and maximum catalyst concentrations were determined, based on which an initial population of 4 possible solutions was formed as

$$X^1=\left(0;10^{-4};2\cdot10^{-4};3\cdot10^{-4}\right). \quad (11)$$

The optimization criterion introduced was a functional expressing the absolute difference between the calculated and the specified conversion value $\widetilde{K}$ at the time moment t_{end}=85 minutes,

$$G(X^*(0))(t_{end})=\left|K(t_{end})-\widetilde{K}\right|\rightarrow\min. \quad (12)$$

For calculating the conversion, an expression reflecting the extent of monomer consumption was used.

$$K=\frac{[M_0]-[M]}{[M_0]}\cdot100\%, \quad (13)$$

where $[M_0]$,$[M]$ initial and current monomer concentrations, respectively.

The permissible accuracy for stopping the algorithm was set ε=0.5%. The mutation parameter used was p_m=0.2.

The iterative execution of the steps of the described genetic algorithm allowed the identification of the desired catalyst concentration, which was determined to be $1.033{\cdot}10^{-4}$ mol/L.

Stage 2. To achieve a product with the specified average molecular weight $\widetilde{M_w}$ = $680{\cdot}10^3$ g/mol, the problem of finding the concentration of diisobutylaluminum hydride was solved at a fixed catalyst dosage found during the implementation of Stage 1.

The optimization criterion introduced was the absolute difference between the calculated and specified values of the average molecular weight

$$G(X^*(0))(t_{end})=\left|M_w(t_{end})-\widetilde{M_w}\right|\rightarrow min. \quad (14)$$

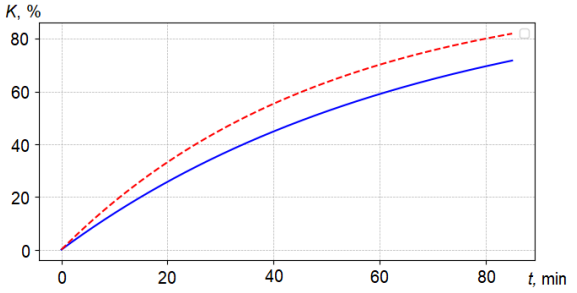


Figure 4. The relationship between conversion and time for various compositions of the reaction mixture (the dashed line represents the initial composition, and the solid line represents the optimal composition).

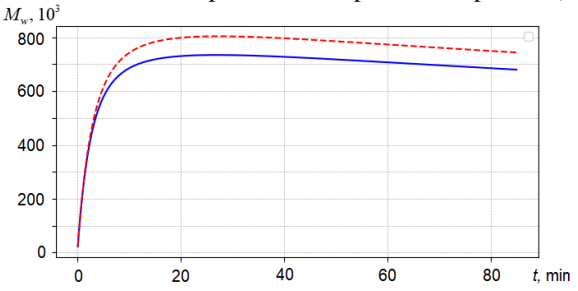


Figure 5. The dependence of the average molecular weight on time for different compositions of the reaction mixture (the dashed line represents the initial composition, and the solid line represents the optimal composition).

The initial population of possible solutions was formed as a vector of values $X^2 = (0; 2 \cdot 10^{-4}; 4 \cdot 10^{-4}; 6 \cdot 10^{-4})$. Given the constant molar ratio $NdCl_3$/TIBA/piperylene = 1 mol/12 mol/2 mol, it follows that the concentration of TIBA is 12 times higher than the value of the found catalyst concentration and is $12.4 \cdot 10^{-4}$ for further computation. The permissible accuracy for solving the problem was set to $\varepsilon = 10^3$. The mutation parameter used was $p_m = 0.2$.

The iterative execution of the described genetic algorithm allowed for the identification of the concentration value of diisobutylaluminum hydride, equal to $3.67 \cdot 10^{-4}$ mol/L. To assess the correctness of the found concentration values of the starting reagents, a computational experiment was conducted to visualize the obtained dependencies (Figures 4-5).

The analysis of the figures reveals that the found optimal composition of reagents (monomer – 1.39 mol/L, catalyst – $1.033 \cdot 10^{-4}$ mol/L; diisobutylaluminum hydride (DIBAH) – $3.67 \cdot 10^{-4}$ mol/L; triisobutylaluminum (TIBA) – $1.68 \cdot 10^{-3}$ mol/L) contributes to achieving conversion values of 72% and an average molecular weight of $680 \cdot 10^3$ g/mol for the resulting polymer product at 85 minutes of model time.

Questions regarding the numerical assessment of the influence of diisobutylaluminum hydride concentration on the values of average molecular characteristics have been raised previously in several studies. In study (Miftakhov *et al.*, 2021), focused on the analysis of continuous production of 1,4-cis-polyisoprene, it was shown that reducing the dosage of organoaluminum compounds leads to an increase in average molecular characteristics. Specifically, decreasing the dosage of diisobutylaluminum hydride from 100% to 10% of the initial molar concentration resulted in an increase in the weight-average molecular weight from $771 \cdot 10^3$ g/mol to $922 \cdot 10^3$ g/mol. Thus, varying the concentration of diisobutylaluminum hydride within a certain range of the initial molar concentration of reagents allows control over the molecular weight of the resulting product. Such moderate changes also indicate that the mechanism of polymer chain termination due to interaction with diisobutylaluminum hydride is not the only one; the interaction with triisobutylaluminum, initially present in the system as part of the catalytic complex, has a significant impact on termination. In another work (Antipina *et al.*, 2020), the issue of determining the dosage of diisobutylaluminum hydride to achieve a weight-average molecular weight of $6 \cdot 10^5$ g/mol at a conversion of 80% was addressed. The found concentration of diisobutylaluminum hydride, $3.78 \cdot 10^{-4}$ mol/L, agrees with the results obtained in this study.

The solution to the problem of finding the optimal composition of the reaction mixture was conducted step by step; however, the genetic algorithm effectively handles multi-factor optimization tasks not only in continuous but also in discrete variable spaces. Such a need often arises when optimizing technological parameters in industrial production, where the range of their possible values is limited. In this case, the use of heuristic optimization methods is the only way to solve the problem.

Conclusions

Thus, a numerical algorithm has been developed to solve the problem of finding the optimal composition of the initial reaction mixture using a heuristic optimization method, and its effectiveness has been evaluated using the example of the process of obtaining 1,4-cis-polyisoprene in the presence of a neodymium-based catalyst.

The method of solution and its software implementation are based on a genetic algorithm, which relies on creating a population of potential solutions using probabilistic laws. Despite the abundance of classical optimization methods embedded in the functionality of popular programming environments, the genetic algorithm proves preferable in the exploration and optimization

of complex multifactor physicochemical systems. This preference stems from its ability to find the global optimum due to the stochastic nature of solution search and the ability to maintain diversity within the population.

The software implementation of this algorithm and the conducted computational experiments have allowed for the identification of the initial composition of the reaction mixture conducive to obtaining a product with the specified characteristics. The presented research methodology can be utilized in investigating similar processes based on the polymerization principle, and the developed numerical algorithm can be applied in the case of multifactor optimization.

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