SCIENTIFIC CONFERENCE

Russian Supercomputing Days

Parallel computing in solving the problem of interval multicriteria optimization in chemical kinetics

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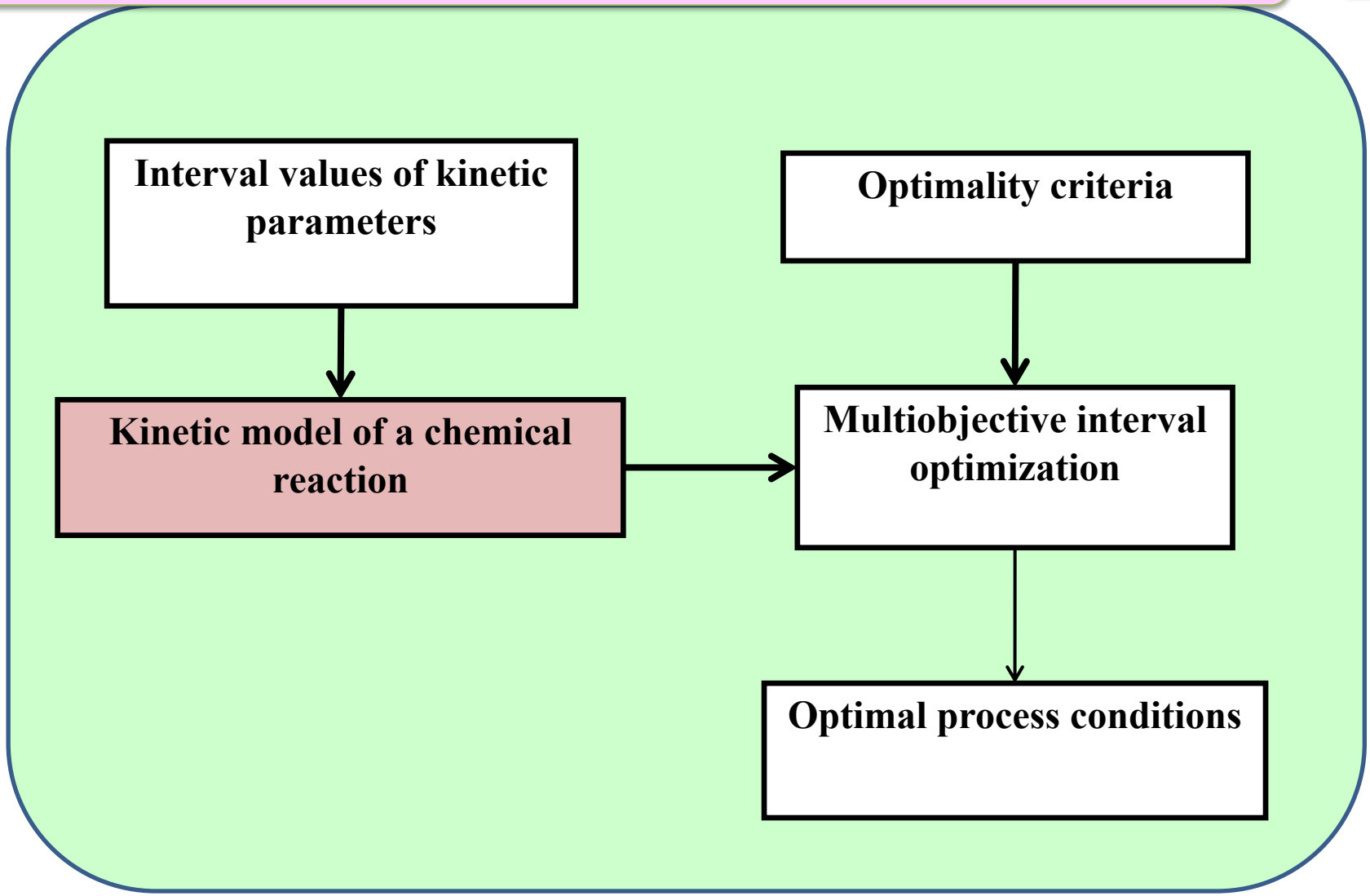
Actuality


Interval values of kinetic parameters
Optimality criteria
Kinetic model of a chemical reaction
Multiobjective interval optimization
Optimal process conditions

Interval Analysis Methods

Replacement in the algorithm of the numerical method of all arithmetic operations and functions on real numbers by their interval analogs

→ Moore effect - an excessive increase in the width of the interval solution compared to the true

Two-way method for solving an interval kinetic problem*

*Dobronets, B.S. Interval mathematics. Tutorial. Krasnoyar. State. Univ., 216 p. (2004).
Bukhtoyarov, S.E., Emelichev, V.A. Parametrization of the optimality principle (from Pareto to Slater) and stability of multicriteria trajectory problems. J. Appl. Ind. Math 10(2), 3–18 (2003).

Moore Effect Demonstration*

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$w_1 = k_1 x_1$$
$$w_2 = k_2 x_2$$
$$t \epsilon [0; 5]$$
$$x_1 = [1; 1]$$
$$x_2 = x_3 = [0; 0]$$

$$\begin{cases} \frac{dx_1}{dt} = -\omega_1 = -k_1 x_1, \\ \frac{dx_2}{dt} = \omega_1 - \omega_2 = k_1 x_1 - k_2 x_2, \\ \frac{dx_3}{dt} = \omega_2 = k_2 x_2, \end{cases}$$

$$\boldsymbol{k}_1 = [0.2231; 1.164], \ \boldsymbol{k}_2 = [0.2369; 1.236].$$

$$x_1(0) = x_1^0, \quad x_2(0) = x_2^0, \quad x_3(0) = x_3^0.$$

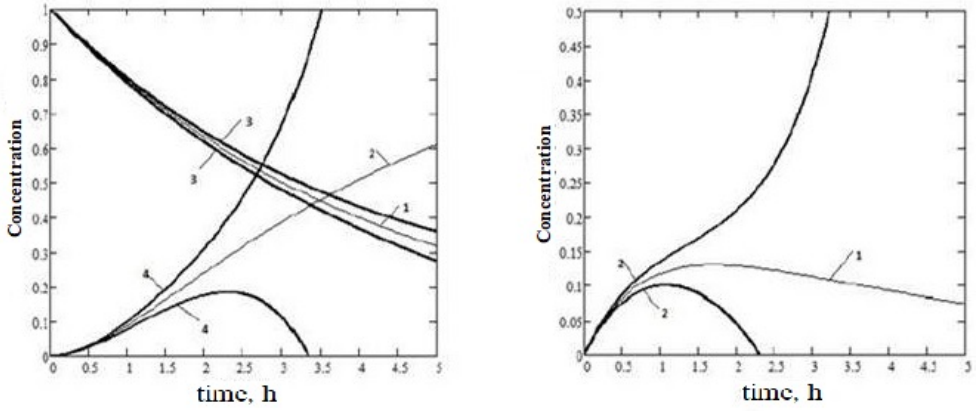


Fig. a) 1,2 - average values for A,C; 3,4 - two-sided restrictions for A,C;
b) 1 - average value for B; 2 - two-sided restriction for B;

**Bulatov I.M., Mustafina S.A. Construction of a mathematical model of the process of obtaining phthalic anhydride by methods of interval analysis. In the collection: MATHEMATICAL MODELING OF PROCESSES AND SYSTEMS. Proceedings of the V All-Russian Scientific and Practical Conference dedicated to the 110th anniversary of Academician A.N. Tikhonov. 2016. S. 98-101.*

Mathematical model. Two-sided method for solving the interval problem

$$\frac{dy_i}{dt} = \varphi_i(y_i, k_j), \quad i = 1,...,I, \quad j = 1,...,J, \tag{1}$$

$$k_j = k_j^0 \exp(-\frac{E_j}{RT}) \tag{2}$$

$y_i(0) = y_i^0, \quad t \in [0, t^*],$

where y_i – concentration of chemical reaction substances, mol/l; t^*- reaction time, min; φ_i- functions of the right parts according to the rate of reaction steps; I- number of chemical reaction substances; J- number of chemical reaction stages; k_j- stage rate constants; k_j^0- pre-exponential factors; E_j- activation energy of stages, kcal/mol; R - universal gas constant, 2 cal/(mol*K); T- temperature, K.

$$T \in (\underline{T}, \overline{T}) \Rightarrow k_j \in (\underline{k_j}, \overline{k_j})$$

y_i isotone by parameter k_j , if $\frac{\partial \varphi_i}{\partial k_j} > 0$ (3)

y_i antiton by parameter k_j , if $\frac{\partial \varphi_i}{\partial k_j} < 0$ (4)

otherwise φ_i does not depend on k_j .

$$y_i \in (\underline{y_i}, \overline{y_i})$$

Kinetic model of the catalytic reaction for the synthesis of benzylalkyl ethers

Table 1. Stages of chemical transformations and values of the kinetic parameters in the catalytic synthesis of benzyl butyl ethers

N	Stages of chemical transformations	E_j	$\ln k_j^0$
1.	$PhCH_2OH(Y_1) + CuBr_2(Y_2) \rightarrow [PhCH_2]^+[CuBr_2(OH)]^-(Y_3)$	5.40	7.00
2.	$[PhCH_2]^+[CuBr_2(OH)]^-(Y_3) + BuOH(Y_4) \rightarrow [PhCH_2OBu]H^+ [CuBr_2(OH)]^-(Y_5)$	12.2	15.4
3.	$[PhCH_2OBu]H^+ [CuBr_2(OH)]^-(Y_5) \rightarrow PhCH_2OBu(Y_6) + H_2O(Y_7) + CuBr_2(Y_2)$	10.3	9.50
4.	$[PhCH_2]^+[CuBr_2(OH)]^-(Y_3) + PhCH_2OH(Y_1) \rightarrow [PhCH_2OHCH_2Ph]^+ [CuBr_2(OH)]^-(Y_8)$	14.0	17.6
5.	$[PhCH_2OHCH_2Ph]^+ [CuBr_2(OH)]^-(Y_8) \rightarrow PhCH_2OCH_2Ph\,(Y_9) + H_2O(Y_7) + CuBr_2(Y_2)$	21.7	24.1
6.	$BuOH(Y_4) + CuBr_2(Y_2) \rightarrow [Bu]^+[CuBr_2(OH)]^-\,(Y_{10})$	15.0	10.7
7.	$[Bu]^+[CuBr_2(OH)]^-\,(Y_{10}) + BuOH(Y_4) \rightarrow [BuOHBu]^+[CuBr_2(OH)]^-\,(Y_{11})$	18.5	20.4
8.	$[BuOHBu]^+[CuBr_2(OH)]^-\,(Y_{11}) \rightarrow BuOBu(Y_{12}) + H_2O(Y_7) + CuBr_2(Y_2)$	35.1	34.1
9.	$[Bu]^+[CuBr_2(OH)]^-\,(Y_{10}) + PhCH_2OH(Y_1) \rightarrow [PhCH_2OBu]H^+ [CuBr_2(OH)]^-(Y_5)$	11.9	12.4

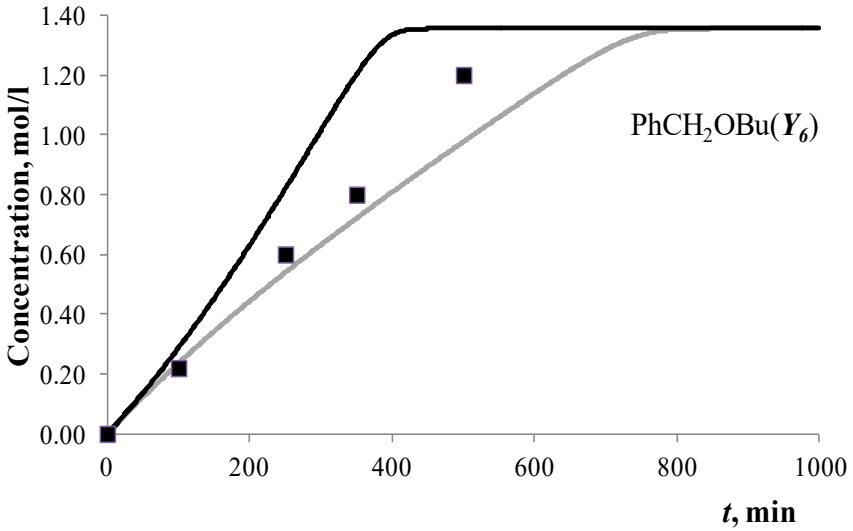
K. F. Koledina, I. M. Gubaidullin, S. N. Koledin, A. R. Baiguzina,L. I. Gallyamovaa, and R. I. Khusnutdinov Kinetics and Mechanism of the Synthesis of Benzylbutyl Ether in the Presence of Copper-Containing Catalysts // Russian Journal of Physical Chemistry A, 2019, Vol. 93, No. 11, pp. 2146–2151.

Interval mathematical model of the catalytic reaction for the synthesis of benzylalkyl ethers

$$
\begin{cases}
\dfrac{d\underline{y_1}}{dt} = -\bar{k}_1 \underline{y_1}\underline{y_2} - \bar{k}_4 \underline{y_3}\underline{y_1} - \bar{k}_9 \underline{y_1}\underline{y_{10}}; \\
\dfrac{d\underline{y_2}}{dt} = -\bar{k}_1 \underline{y_1}\underline{y_2} + \underline{k_3}\underline{y_5} + \underline{k_5}\underline{y_8} + \underline{k_8}\underline{y_{11}}; \\
\dfrac{d\underline{y_3}}{dt} = \underline{k_1}\underline{y_1}\underline{y_2} + \bar{k}_2 \underline{y_3}\underline{y_4} - \bar{k}_4 \underline{y_3}\underline{y_1}; \\
\dfrac{d\underline{y_4}}{dt} = -\bar{k}_2 \underline{y_3}\underline{y_4} + \bar{k}_6 \underline{y_2}\underline{y_4} - \bar{k}_7 \underline{y_{10}}\underline{y_4}; \\
\dfrac{d\underline{y_5}}{dt} = \underline{k_2}\underline{y_3}\underline{y_4} - \bar{k}_3 \underline{y_5} + \underline{k_9}\underline{y_{10}}\underline{y_1}; \\
\dfrac{d\underline{y_6}}{dt} = \underline{k_3}\underline{y_5}; \\
\dfrac{d\underline{y_7}}{dt} = \underline{k_3}\underline{y_5} + \underline{k_5}\underline{y_8} + \underline{k_8}\underline{y_{11}}; \\
\dfrac{d\underline{y_8}}{dt} = \underline{k_4}\underline{y_3}\underline{y_1} - \bar{k}_5 \underline{y_8}; \\
\dfrac{d\underline{y_9}}{dt} = \underline{k_5}\underline{y_8}; \\
\dfrac{d\underline{y_{10}}}{dt} = \underline{k_6}\underline{y_2}\underline{y_4} - \bar{k}_7 \underline{y_{10}}\underline{y_4} - \bar{k}_9 \underline{y_1}\underline{y_{10}}; \\
\dfrac{d\underline{y_{11}}}{dt} = \underline{k_7}\underline{y_{10}}\underline{y_4} - \bar{k}_8 \underline{y_{11}}; \\
\dfrac{d\underline{y_{12}}}{dt} = \underline{k_8}\underline{y_{11}};
\end{cases}
\qquad
\begin{cases}
\dfrac{d\overline{y_1}}{dt} = -\underline{k_1}\overline{y_1}\,\overline{y_2} - \underline{k_4}\overline{y_3}\,\overline{y_1} - \underline{k_9}\overline{y_1}\,\overline{y_{10}}; \\
\dfrac{d\overline{y_2}}{dt} = -\underline{k_1}\overline{y_1}\,\overline{y_2} + \bar{k}_3 \overline{y_5} + \bar{k}_5 \overline{y_8} + \bar{k}_8 \overline{y_{11}}; \\
\dfrac{d\overline{y_3}}{dt} = \bar{k}_1 \overline{y_1}\,\overline{y_2} + \underline{k_2}\overline{y_3}\,\overline{y_4} - \underline{k_4}\overline{y_3}\,\overline{y_1}; \\
\dfrac{d\overline{y_4}}{dt} = -\underline{k_2}\overline{y_3}\,\overline{y_4} + \underline{k_6}\overline{y_2}\,\overline{y_4} - \underline{k_7}\overline{y_{10}}\,\overline{y_4}; \\
\dfrac{d\overline{y_5}}{dt} = \bar{k}_2 \overline{y_3}\,\overline{y_4} - \underline{k_3}\overline{y_5} + \bar{k}_9 \overline{y_{10}}\,\overline{y_1}; \\
\dfrac{d\overline{y_6}}{dt} = \bar{k}_3 \overline{y_5}; \\
\dfrac{d\overline{y_7}}{dt} = \bar{k}_3 \overline{y_5} + \bar{k}_5 \overline{y_8} + \bar{k}_8 \overline{y_{11}}; \\
\dfrac{d\overline{y_8}}{dt} = \bar{k}_4 \overline{y_3}\,\overline{y_1} - \underline{k_5}\overline{y_8}; \\
\dfrac{d\overline{y_9}}{dt} = \bar{k}_5 \overline{y_8}; \\
\dfrac{d\overline{y_{10}}}{dt} = \bar{k}_6 \overline{y_2}\,\overline{y_4} - \underline{k_7}\overline{y_{10}}\,\overline{y_4} - \underline{k_9}\overline{y_{10}}\,\overline{y_1}; \\
\dfrac{d\overline{y_{11}}}{dt} = \bar{k}_7 \overline{y_{10}}\,\overline{y_4} - \underline{k_8}\overline{y_{11}}; \\
\dfrac{d\overline{y_{12}}}{dt} = \bar{k}_8 \overline{y_{11}};
\end{cases}
$$

$$
\underline{y_i}(0) = \overline{y_i}(0) = y_i^0, \quad t \in [0, t^*],
$$

Direct problem solution



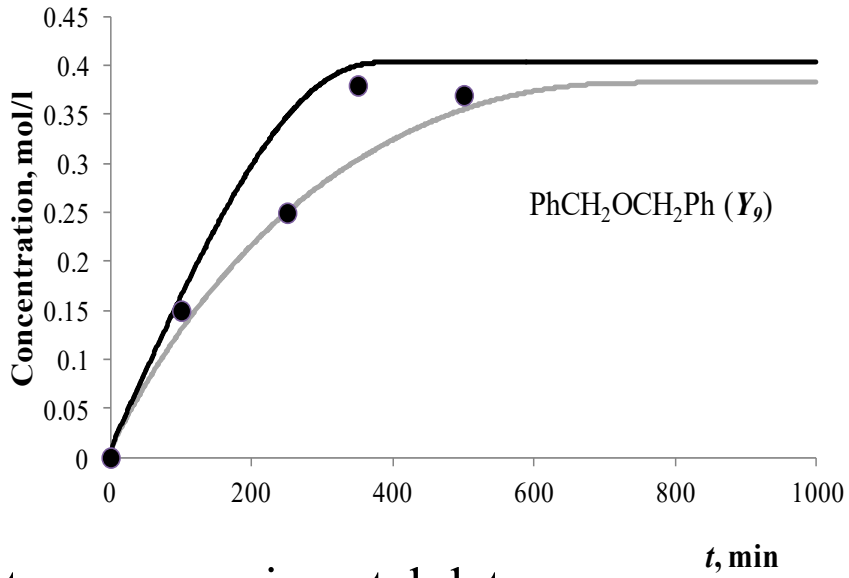


Fig. Correspondence graphs between experimental data (dots) and intervals of calculated values (lines) of changes in the concentration of observed substrates in the temperature range [160ºC, 175ºC] in the reaction of the synthesis of benzyl butyl ethers (average values of the experimental concentrations of the components are given)

Statement of the multi-criteria interval optimization problem

Variable parameter vector

$$X=(x_1, x_2, x_3, x_4, x_5, \ldots),$$

x_1 – reaction temperature; x_2 – initial concentrations of reagents; x_3 – reaction time; x_4 – type of catalyst; x_5 – catalyst supply, etc.

Direct restrictions on variable parameters

$$X \in [X^{\min}, X^{\max}]: x_1 \in [x_1^-, x_1^+]; x_2 \in [x_2^-, x_2^+]; x_3 \in [x_3^-, x_3^+]; x_4 \in [x_4^-, x_4^+];$$

$$x_5 \in [x_5^-, x_5^+];\ldots.$$

Vector function of optimality criteria

$$F(X)=(f_1(X), f_2(X), f_3(X), \ldots)$$

Then the maximization (minimization similarly, with a "-" sign) of the optimality criteria in the area D_X can be written as

$$\max_{X \in D_X} F(X) = F(X^*) = F^*$$

Multi-criteria interval optimization problem for the catalytic reaction of benzylbutyl ether synthesis

- Variable parameter vector $X=(x_1, x_2)$, where x_1 – reaction temperature, T; x_2 – temperature change radius.

- Vector function of optimality criteria $F(X)=(f_1(X), f_2(X))$:

$$f_1(X) = y_{PhCH_2OBu(Y_6)}(t^*, T, N) \rightarrow \max \quad (3)$$

$$f_2(X) = y_{PhCH_2OCH_2Ph(Y_9)}(t^*, T, N) \rightarrow \min \quad (4)$$

$$mid\ f_l = \frac{\underline{f_l} + \overline{f_l}}{2} \quad \text{– interval midpoint} \quad (5)$$

$$wid\ f_l = \overline{f_l} - \underline{f_l} \quad \text{– interval width} \quad (6)$$

Parallel scheme for implementing the computational process

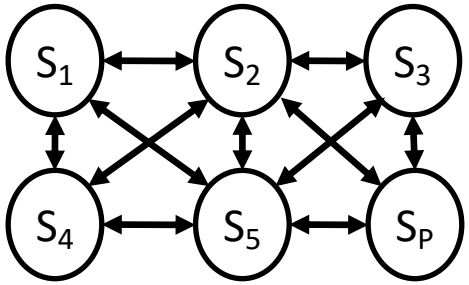


Fig. Island parallelization model for solving the multi-criteria optimization problem

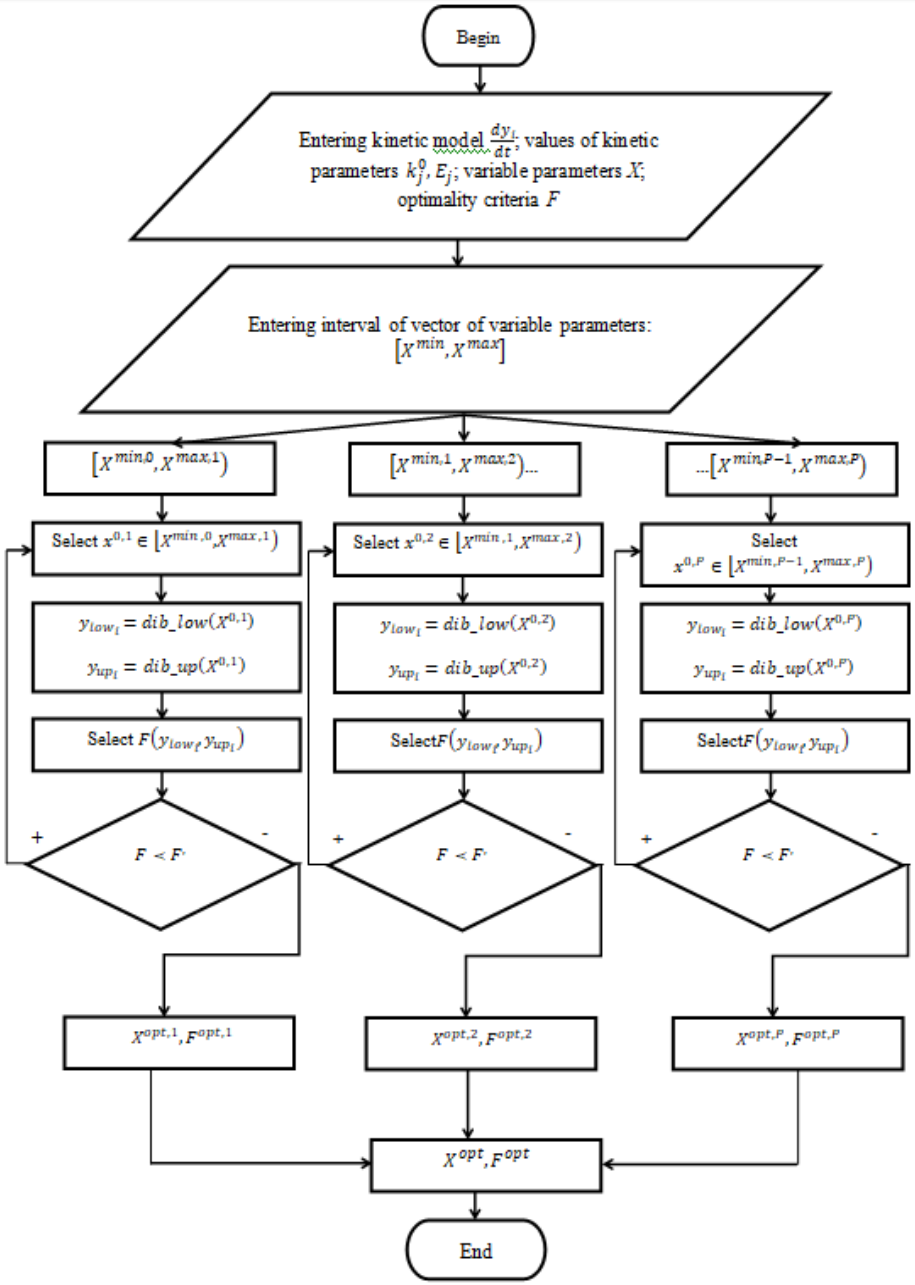
$$S = \bigcup_{i=1}^{|P|} S_i$$

where S – multipopulation, S_i – subpopulations (islands), $|P|$ - number of processors.

$$\left[x_i^{min}, x_i^{max}\right] = \left[x_i^{min,0}, x_i^{max,1}\right) \cup \left[x_i^{min,1}, x_i^{max,2}\right) \cup \ldots \cup \left[x_i^{min,P-1}, x_i^{max,P}\right),$$

$$i = 1,2, \ldots I$$

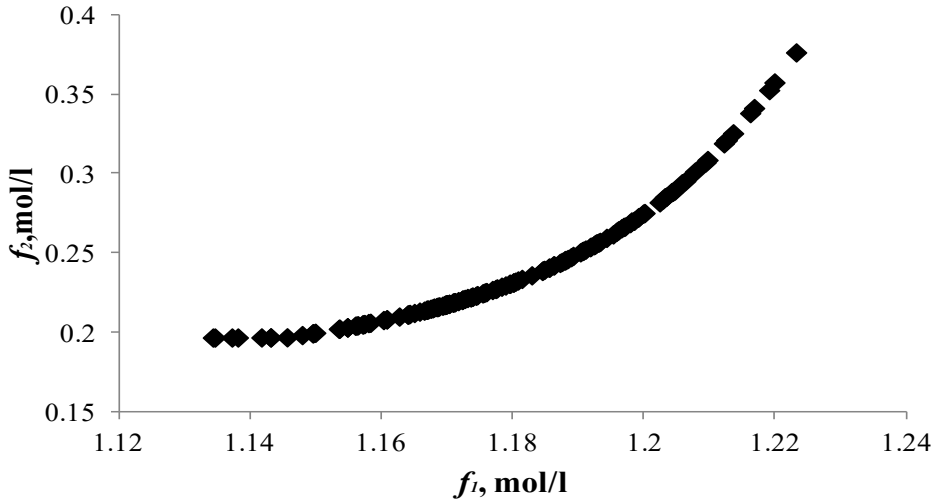
Scheme for parallelizing the computational process for solving the problem of interval multicriteria optimization in chemical kinetics



Research results

The catalytic reaction of the synthesis of benzylbutyl ether

$x_1 \in [160, 175]$ $x_2 \in [1, 5]$



The evolutionary algorithm of multiobjective optimization NSGA-II (Non-dominated Sorting Genetic Algorithm)

Fig. Approximation of the Pareto front of the MCO problem for the catalytic reaction of the synthesis of benzyl butyl ether

Research results

4-core PC Intel Core i7-8550U CPU, RAM 16GB, OS Windows10, Software system: Matlab (MATrix LABoratore). The Parallel Computing Toolbox with OpenMP was used.

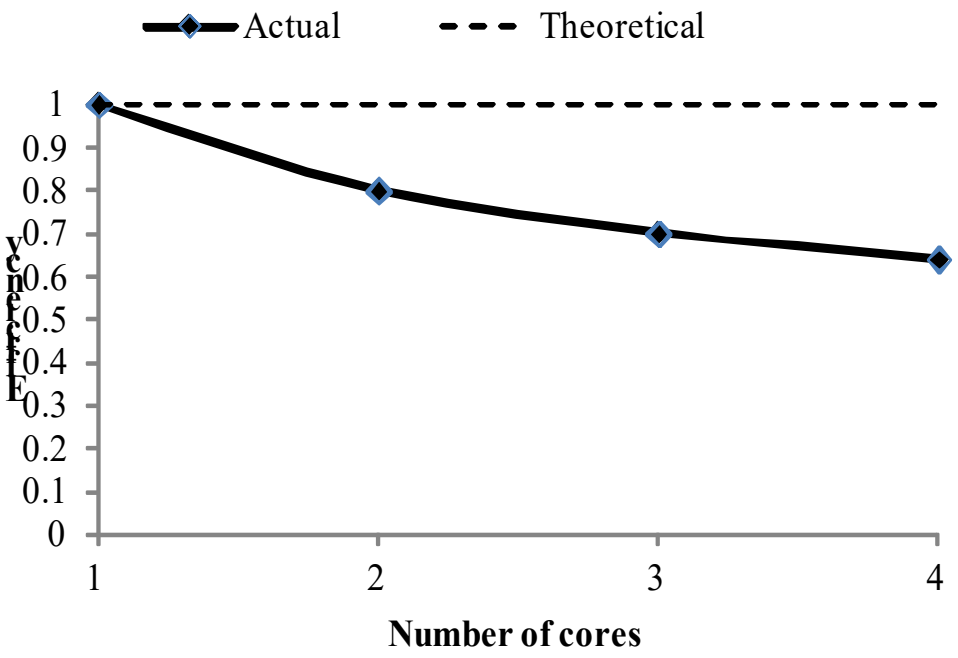


Fig. Efficiency of the parallel program for solving the interval MCO-task of catalytic synthesis of benzylbutyl ether

Conclusion

- A statement of the problem of interval multicriteria optimization of the conditions of a multistage reaction based on a kinetic model has been developed.

- The solution of the MCO interval problem was obtained by varying the temperature from 160ºC to 175ºC, with a temperature spread of no more than 5ºC. An increase in temperature leads to an increase in the yield of the target product, but the concentration of the by-product also increases.

- A parallel scheme has been developed for solving the interval problem of the MCO and an assessment of the efficiency of the execution of the parallel program has been carried out. The efficiency of the developed parallelization algorithm was 68%.

Thank you for attention!

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