Parallel Computing in Solving the Problem of Interval Multicriteria Optimization in Chemical Kinetics

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Abstract. Interval multi-criteria optimization (MCO) of the conditions based on the kinetic model is relevant for both laboratory and industrial processes. In the work for the laboratory catalytic reaction of the synthesis of benzylbutyl ether, the problem of interval MCO of the conditions of conducting based on a kinetic model is solved. The problem was solved in the form of Pareto approximation using the evolutionary algorithm of multiobjective optimization NSGA-II and parallel computing. The solution of the MCO interval problem was obtained by varying the temperature from 160 °C to 175 °C, with a temperature spread of no more than 5 °C. 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.

Keywords: Parallel computing · Interval multicriteria optimization · Chemical kinetics · Benzylbutyl ether

1 Introduction

The basis for optimizing the conditions of complex chemical processes is their kinetic model. The kinetic model reflects the regularities of the reaction, the effect of the conditions on the reaction rate, on the yield of target and by-products and reaction time. In a complex chemical process, including the process of oil production [1], oil refining, it is difficult to single out one optimization criterion. Often several criteria are set, which may be contradictory and have different dimensions. Such a task is defined as multi-criteria optimization. Due to the fact that in practice it is difficult to maintain the calculated exact optimal mode of the process, it is necessary to select the optimal interval of conditions [2]. Which requires solving the problem of interval multi-criteria optimization, including the development of an interval kinetic model [3, 4]. The range of variation of the conditions can be quite wide when searching for the optimal solution, and the dimension of the mathematical model can reach several dozen differential equations in the number

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of reaction components, so it is relevant to develop a parallel calculation scheme when solving the problem of interval multicriteria optimization in chemical kinetics.

The object of the study is the catalytic reaction of the synthesis of benzylalkyl esters, namely benzylbutyl ether. The catalytic reaction of the synthesis of benzylalkyl esters occurs by intermolecular dehydration of benzyl and n-butyl alcohols with the formation of three esters: target benzylbutyl and side dibenzyl, dibutyl [5, 6]. The development of a detailed kinetic model will solve the problem of multi-criteria optimization of the reaction conditions in order to maximize the target yield and minimize the output of by-products.

2 Mathematical Model

The mathematical model of the kinetics of complex chemical reactions in the form of a system of ordinary nonlinear differential equations (SONDE) has the form [7]:

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

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

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

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.

When calculating a task with interval values of the process temperature $T \in (\underline{T}, \overline{T})$, the rate constants of the stages will have interval values according to (2) $k_j \in (\underline{k_j}, \overline{k_j})$. To solve the system of differential Eqs. (1), a two-sided method for solving the interval problem will be used [8, 9]. For each component y_i it is possible to introduce a dependence on the boundaries of kinetic parameters: y_i isotone by parameter k_j, if $\frac{\partial \varphi_i}{\partial k_j} > 0$ and antiton by k_j, if $\frac{\partial \varphi_i}{\partial k_j} < 0$, otherwise φ_i does not depend on k_j.

Then, accordingly, it is possible to define two systems of differential equations of the form (1) for the lower bound of the concentration change $\underline{y_i}$ – dib_low and for the upper bound $\overline{y_i}$- dib_up.

3 Interval Mathematical Model of the Catalytic Reaction for the Synthesis of Benzylalkyl Ethers

Benzyl butyl ether is widely used as a flavoring agent in various industries. Is a large-capacity, industrial product [6]. The preparation of esters in the reaction of dehydration of benzyl alcohol is best carried out in the presence of catalysts containing copper, in particular $CuBr_2$ [10].

Table 1 shows the stages of chemical transformations and the values of the kinetic parameters of the stages, calculated in the works [11].

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

The mathematical model using the two-sided method for solving the interval problem will have the form of two SONDE for calculating the lower and upper limits of the concentrations of the components (3).

The direct interval kinetic problem was solved using the two-sided method in combination with the multi-step Gear method of variable order [12]. The scheme of chemical transformations of the reaction and the corresponding ranges of values of kinetic

parameters are given in Table 1.

$$
\begin{cases}
\dfrac{d\underline{y_1}}{dt} = -\overline{k}_1\underline{y_1y_2} - \overline{k}_4\underline{y_3y_1} - \overline{k}_9\underline{y_1y_{10}};\\
\dfrac{d\underline{y_2}}{dt} = -\overline{k}_1\underline{y_1y_2} + \underline{k_3y_5} + \underline{k_5y_8} + \underline{k_8y_{11}};\\
\dfrac{d\underline{y_3}}{dt} = \underline{k_1y_1y_2} + \overline{k}_2\underline{y_3y_4} - \overline{k}_4\underline{y_3y_1};\\
\dfrac{d\underline{y_4}}{dt} = -\overline{k}_2\underline{y_3y_4} + \overline{k}_6\underline{y_2y_4} - \overline{k}_7\underline{y_{10}y_4};\\
\dfrac{d\underline{y_5}}{dt} = \underline{k_2y_3y_4} - \overline{k}_3\underline{y_5} + \underline{k_9y_{10}y_1};\\
\dfrac{d\underline{y_6}}{dt} = \underline{k_3y_5};\\
\dfrac{d\underline{y_7}}{dt} = \underline{k_3y_5} + \underline{k_5y_8} + \underline{k_8y_{11}};\\
\dfrac{d\underline{y_8}}{dt} = \underline{k_4y_3y_1} - \overline{k}_5\underline{y_8};\\
\dfrac{d\underline{y_9}}{dt} = \underline{k_5y_8};\\
\dfrac{d\underline{y_{10}}}{dt} = \underline{k_6y_2y_4} - \overline{k}_7\underline{y_{10}y_4} - \overline{k}_9\underline{y_1y_{10}};\\
\dfrac{d\underline{y_{11}}}{dt} = \underline{k_7y_{10}y_4} - \overline{k}_8\underline{y_{11}};\\
\dfrac{d\underline{y_{12}}}{dt} = \underline{k_8y_{11}};
\end{cases}
\qquad
\begin{cases}
\dfrac{d\overline{y_1}}{dt} = -\underline{k_1}\overline{y_1y_2} - \underline{k_4}\overline{y_3y_1} - \underline{k_9}\overline{y_1y_{10}};\\
\dfrac{d\overline{y_2}}{dt} = -\underline{k_1}\overline{y_1y_2} + \overline{k}_3\overline{y_5} + \overline{k}_5\overline{y_8} + \overline{k}_8\overline{y_{11}};\\
\dfrac{d\overline{y_3}}{dt} = \overline{k}_1\overline{y_1y_2} + \underline{k_2}\overline{y_3y_4} - \underline{k_4}\overline{y_3y_1};\\
\dfrac{d\overline{y_4}}{dt} = -\underline{k_2}\overline{y_3y_4} + \underline{k_6}\overline{y_2y_4} - \underline{k_7}\overline{y_{10}y_4};\\
\dfrac{d\overline{y_5}}{dt} = \overline{k}_2\overline{y_3y_4} - \underline{k_3}\overline{y_5} + \overline{k}_9\overline{y_{10}y_1};\\
\dfrac{d\overline{y_6}}{dt} = \overline{k}_3\overline{y_5};\\
\dfrac{d\overline{y_7}}{dt} = \overline{k}_3\overline{y_5} + \overline{k}_5\overline{y_8} + \overline{k}_8\overline{y_{11}};\\
\dfrac{d\overline{y_8}}{dt} = \overline{k}_4\overline{y_3y_1} - \underline{k_5}\overline{y_8};\\
\dfrac{d\overline{y_9}}{dt} = \overline{k}_5\overline{y_8};\\
\dfrac{d\overline{y_{10}}}{dt} = \overline{k}_6\overline{y_2y_4} - \underline{k_7}\overline{y_{10}y_4} - \underline{k_9}\overline{y_{10}y_1};\\
\dfrac{d\overline{y_{11}}}{dt} = \overline{k}_7\overline{y_{10}y_4} - \underline{k_8}\overline{y_{11}};\\
\dfrac{d\overline{y_{12}}}{dt} = \overline{k}_8\overline{y_{11}};
\end{cases}
$$

$$
\underline{y_i}(0) = \overline{y_i}(0) = y_i^0, \quad t \in [0, t*], \tag{3}
$$

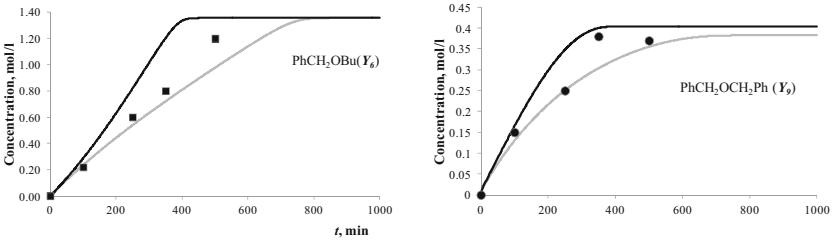

Fig. 1. Correspondence graphs between experimental data (dots) and intervals of calculated values (lines) of changes in the concentration of observed substrates in the temperature range [160 °C, 175 °C] in the reaction of the synthesis of benzyl butyl ethers (average values of the experimental concentrations of the components are given)

Figure 1 shows the correspondence of the experimental data with the intervals of calculated values of the measured substrates of the catalytic reaction of the synthesis of benzyl butyl ethers. The observed substrates are the target reaction product benzylbutyl ether $PhCH_2OBu(Y_6)$ and reaction by-product dibenzyl ether $PhCH_2OCH_2Ph\,(Y_9)$. The

graphs show the values of concentrations in the temperature range [160 °C, 175 °C]. Experimental data on component concentrations are included in the calculated interval (Fig. 1). Thus, the interval values of the parameters obtained for the given temperature intervals describe the experimental data within the error. This gives grounds to conclude that this mechanism is reliable for the catalytic reaction of the synthesis of benzyl butyl ethers when using interval values of variable parameters.

The subsequent introduction of the process into production requires determining the optimal reaction conditions in order to obtain the highest yield of the target benzyl butyl ether PhCH2OBu(Y6) and the smallest by-product of dibenzyl ether PhCH2OCH2Ph (Y9). Based on the values of the kinetic parameters, it is possible to formulate a multicriteria interval optimization problem [13–15].

4 Statement of the Multi-criteria Interval Optimization Problem

Statement and solution of the optimization problem requires the definition of optimality criteria. It is also necessary to define variable parameters and restrictions on them. The process in the optimization problem is a chemical reaction. In chemical technology, such parameters can be: reaction temperature, pressure, initial concentrations of reagents, type of catalyst, reaction time. Restrictions on variable parameters are determined by the nature of the process and technical capabilities.

The mathematical model of problems of chemical kinetics has the form of a system of nonlinear differential equations for changing the concentration of reaction substances. The change occurs in time with known values of kinetic parameters: pre-exponential factors and activation energies of the rates of stages (1).

To determine the optimal conditions for the reaction, it is necessary to solve the problem of multicriteria optimization according to the set optimality criteria, using the described model.

The mathematical formulation of the MCO problem of the conditions of the chemical process according to the kinetic model has the form [14]:

Variable parameter vector

$$X = (x_1,\ x_2,\ x_3,\ x_4,\ x_5,\ \ldots), \tag{4}$$

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

$$F(X) = (f_1(X),\ f_2(X),\ f_3(X),\ \ldots) \tag{5}$$

Then the maximization (minimization similarly, with a "–" sign) of the optimality criteria in the area DX can be written as [15]

$$\max_{X \in D_X} F(X) = F(X^*) = F^* \tag{6}$$

Then the MCO task of the conditions for conducting a catalytic reaction is to determine the values of the variable parameters (4), in order to achieve the extrema of the optimality criteria (5) according to (6).

5 Multi-criteria Interval Optimization Problem for the Catalytic Reaction of Benzylbutyl Ether Synthesis

In the reaction of the synthesis of benzyl butyl ether in the presence of a metal complex catalyst, products are formed $PhCH_2OBu$ (Y_6), $PhCH_2OCH_2Ph$ (Y_9), $BuOBu$ (Y_{12}). Then the task of the MCO of the reaction conditions for the synthesis of benzylbutyl ether has the form:

- Variable parameter vector $X = (x_1, x_2)$, where x_1 – reaction temperature, T; x_2 – temperature change radius.
- Vector function of optimality criteria $F(X) = (f_1(X), f_2(X))$: $f_1(X) = y_{PhCH_2OBu(Y_6)}(t^*, T, N) \to \max$; $f_2(X) = y_{PhCH_2OCH_2Ph(Y_9)}(t^*, T, N) \to \min$.

To solve multicriteria interval optimization, it is necessary to calculate the values of optimality criteria that depend on interval parameters. An interval can be uniquely defined by its midpoint and width.

Then for $F(X)$, $l = 1, 2$:

$$mid\, f_l = \frac{\underline{f_l} + \overline{f_l}}{2} - \text{interval midpoint}, \tag{7}$$

$$wid\ f_l = \overline{f_l} - \underline{f_l} - \text{interval width}. \tag{8}$$

The task of the MCO is to maximize the optimality criteria in the area D_X by (6).

6 Parallel Scheme for Implementing the Computational Process

Work on the development of efficient evolutionary algorithms for solving the problem of multicriteria optimization has been actively carried out in recent decades [16]. The advantages are obtained by methods that take into account the principles of Paretto-dominance based on genetic algorithms. Increasing the performance of computing resources allows for high-performance computing in a reasonable time.

The basis of parallelization of multiobjective optimization algorithms is the decomposition and structuring of the population (a set of possible solutions). That is, the division of the original population into several subsets (subpopulations). Decomposition can be implemented in various ways. Partitioning methods define parallelization models. The most popular parallelization models are: the island parallelization model [17], the global client/server model [18], and the cellular model [19]. The most common model of parallelization of the computational process is the island model of parallelization (Fig. 2).

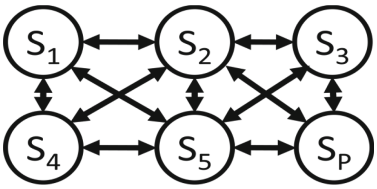

Fig. 2. Island parallelization model for solving the multi-criteria optimization problem

$$S = \bigcup_{i=1}^{|P|} S_i, \tag{9}$$

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

From a multipopulation of values of variable parameters (desired conditions for carrying out a catalytic reaction), subpopulations are created according to the number of available processors. According to Fig. 2 individuals settle on several isolated islands. These subpopulations will develop independently, with subsequent synchronization of results.

This scientific study proposes a modification of the island parallelization model according to the distribution of intervals of variation of kinetic parameters.

If P – the number of available processors, then the intervals of parameter variation can be divided into processors and calculated in parallel (similarly (9)):

$$\left[x_i^{min}, x_i^{max}\right] = \left[x_i^{min,0}, x_i^{max,1}\right) \cup \left[x_i^{min,1}, x_i^{max,2}\right) \cup \cdots \cup \left[x_i^{min,P-1}, x_i^{max,P}\right), \; i = 1, 2, \ldots I, \tag{10}$$

Figure 3 shows the parallelization scheme of the computational process for solving the problem of interval multicriteria optimization in chemical kinetics. The input data are: kinetic model of the process in the form of a system of differential Eqs. (1), values of kinetic parameters - pre-exponential factors and activation energy of stages, a list of variable parameters and optimality criteria. An interval is set for the vector of variable parameters $[X^{\min}, X^{\max}]$. And the corresponding subintervals are distributed among the available processors by (10). For the value (selected using the NSGA-II Pareto approximation algorithm [20]), lower and upper values of component concentrations are calculated from this subinterval using two systems of differential equations for the lower bound *dib_low* and for the upper bound *dib_up*. The values of the optimality criteria (7), (8) are calculated from the concentrations of the components. After checking the nondominability condition of the solution, the optimal value of the vector is determined $X^{opt,p}$ and $F^{opt,p}$ on each subinterval. At the last stage, the total values are calculated X^{opt} and F^{opt} over the entire range of variation.

7 Research Results

For the catalytic reaction of the synthesis of benzylbutyl ether, the effect of the temperature change intervals of the process on the values of the optimality criteria will be

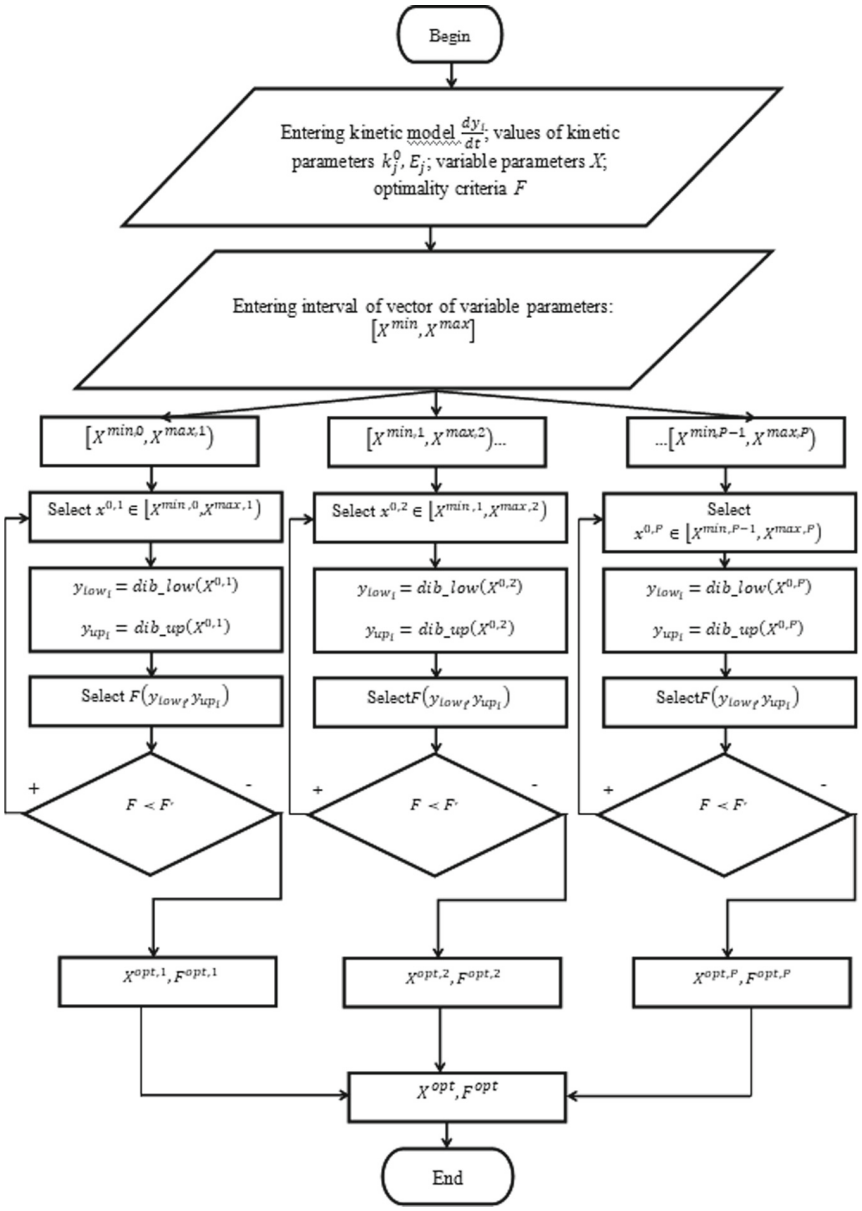

Fig. 3. Scheme for parallelizing the computational process for solving the problem of interval multicriteria optimization in chemical kinetics

calculated. The variable parameters are $x_1 \in [160,\ 175]$; $x_2 \in [1,\ 5]$. Optimization criteria $F(X) = (f_1(X), f_2(X))$. The values of the optimality criteria are subject to restrictions on changing the width of the interval depending on the temperature spread no more

than a given value for each criterion. It is necessary to maximize the optimality criteria according to (10).

The problem was solved in the form of Pareto approximation using the evolutionary algorithm of multiobjective optimization NSGA-II (Non-dominated Sorting Genetic Algorithm) and parallel computing according to the scheme in Fig. 3.

Figure 4 shows the results of solving the problem of MCO of the reaction conditions for the synthesis of benzyl butyl ether in the presence of a metal complex catalyst. The results obtained in Fig. 4 corresponds to a change in temperature from 160 °C to 175 °C (according to the growth of optimization criteria), with a temperature spread of no more than 5 °C. An increase in temperature leads to an increase in the yield of the target product (the average value of the criterion f_1), but the concentration of the by-product also increases (the average value of the criterion f_2). Further choice of a particular solution is up to the decision maker.

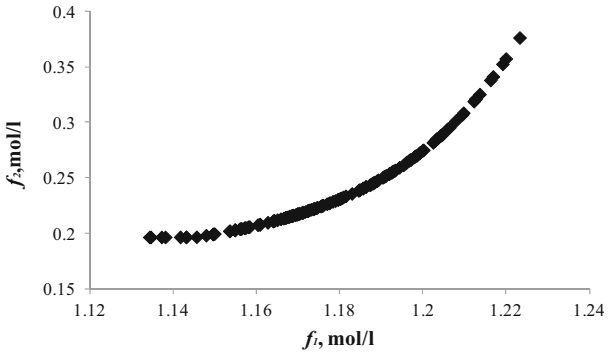

Fig. 4. Approximation of the Pareto front of the MCO problem for the catalytic reaction of the synthesis of benzyl butyl ether

For the calculation, use a 4-core PC Intel Core i7-8550U CPU, RAM 16 GB, OS Windows10, Software system: Matlab (MATrix LABoratore). The Parallel Computing Toolbox with OpenMP was used. Speedup and parallel efficiency are determined to evaluate parallelization. Figure 5 compares the theoretical and calculated efficiency of the parallel program. For the chosen algorithm for parallelizing the computational process for solving the interval MCO problem for the catalytic synthesis of benzyl butyl ether, the parallel efficiency is 68%. However, solving subtasks on different threads by the iterative method can take different times and lead to a noticeable imbalance in calculations.

Perhaps the use of a larger number of cores will make it possible to conduct a computational experiment more efficiently. What will be implemented in further research.

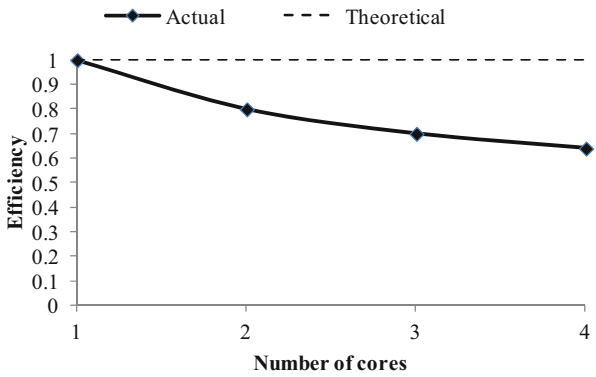

Fig. 5. Efficiency of the parallel program for solving the interval MCO-task of catalytic synthesis of benzylbutyl ether

8 Conclusion

Interval multi-criteria optimization of the conditions based on the kinetic model is relevant for both laboratory and industrial processes. In the work for the laboratory catalytic reaction of the synthesis of benzylbutyl ether, the problem of interval MCO of the conditions of conducting based on a kinetic model is solved. The solution of the MCO interval problem was obtained by varying the temperature from 160 °C to 175 °C, with a temperature spread of no more than 5 °C. 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%. The developed parallel algorithm for solving the interval problem of the MCO will be used to analyze other catalytic industrial and laboratory processes.

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