



Parallel Algorithm for Calculating the Radius of Stability in Multicriteria Optimization Conditions for Catalytic Reforming of Gasoline

Kamila Koledina^{1,2} , Sergey Koledin² ,
and Irek Gubaydullin^{1,2} 

¹ Institute of Petrochemistry and Catalysis of RAS, Ufa, Russia

² Ufa State Petroleum Technological University, Ufa, Russia

Abstract. In the work the problem of multicriteria optimization for reaction conditions of the catalytic reforming of gasoline was solved based on a kinetic model. The criteria of the process optimality are considered, such as minimization of the aromatic hydrocarbons content in the final reformat in accordance with environmental requirements and; maximizing the octane number of the reformat. The problem of analyzing the stability of the Pareto set is formulated. A parallel algorithm for calculating the radius of stability for the solution of the problem of multicriteria optimization with the decomposition of the Pareto set into subsets according to the number of processors is developed. The radius of stability of the optimum temperature values at the reactor inlet was calculated for the catalytic reforming of gasoline. Evaluation of the efficiency of parallel program execution is carried out.

Keywords: Multicriteria optimization · Catalytic reforming of gasoline · Radius of stability · Parallel algorithm for calculating the stability radius

1 Introduction

In the study of chemical kinetics, it is necessary to consider the factors that affect the solution accuracy such as inaccuracy of initial data, inadequacy of models of real processes, error of numerical methods, rounding errors, etc. [1–3]. The problem of chemical reaction conditions optimization is based on a kinetic model. It is impossible to correctly formulate and correctly solve an arbitrary optimization problem without examining it for stability. Complex multistage chemical processes require the determination of the permissible ranges of parameter values that ensure stability of the calculated solution with an acceptable error.

Papers [4, 5] are devoted to assessing the stability of optimal solutions in optimization problems. Stochastic stability which is based on Lyapunov stability was studied. Extreme level of initial perturbation data, under which the solution is Pareto optimal, is possible [6].

In [1], the general formulation and solution of the stability problem for multicriteria trajectory problems is investigated. The type of stability in the problem of independent perturbations in the input data, for which new effective solutions do not appear, is

investigated and also formula for calculating the radius of stability of the problem is determined, necessary and sufficient conditions for stability are indicated [1]. For problems of chemical kinetics, it is necessary to determine the radius of stability for each parameter in order to possibly change the calculated values with an area of a given error while analyzing the stability of multicriteria optimization (MCO). A solution to the problem of multicriteria optimization is the Pareto-set of unimprovable solutions with a sufficiently large power to determine the smoothest solution possible. That is, solutions are determined with no discontinuity and the presence of the maximum number of points. Determining the radius of stability requires solving direct kinetic problems for each solution from the entire Pareto set. Mathematical models of complex, especially industrial processes, have a large dimension and are computationally complex. It is relevant to use parallel algorithms to solve the problem of analyzing the stability of the Pareto set.

The industrial process of catalytic reforming of gasoline is the when analyzing the stability of multicriteria optimization (MCO). The main problems of the catalytic reforming of gasoline are restrictions on the content of benzene and the amount of aromatic hydrocarbons in the final reformate. As a result, a restriction is imposed on the process product in terms of the content of these components. However, the main purpose of the catalytic reforming process is to increase the octane number (ON) of gasoline. Therefore, along with environmental criteria, the octane number of the mixture is the necessary criterion, which value depends on the composition of the product [7]. Therefore, it is relevant to solve the problem of multicriteria optimization of the process conditions.

In this paper, the application of methods for analyzing the stability of multicriteria optimization problems for research industrial catalytic reforming of gasoline with parallelization calculations will be shown.

2 Multicriteria Optimization in Catalytic Reforming of Gasoline Based on a Kinetic Model

The reactor unit of a catalytic reforming process consists of three adiabatic reactors, each of which is supplied with mixture which is heated to the desired temperature. The variable parameters are operating conditions: temperatures at the inlet to the reactor T_j , $j = 1, 2, 3$. Vector variable parameters $X = (x_1, x_2, x_3)$, where $x_1 = T_1$; $x_2 = T_2$; $x_3 = T_3$.

The complex industrial process of catalytic reforming of gasoline is characterized by the following optimality criteria [8]:

- 1) The main criterion of optimality for the catalytic reforming of gasoline is an increase in the octane number (ON_i) of the reformate. In the calculations, octane number additivity of the mixture components is allowed. Then

$$f_1(X) = \sum_{i=1}^l y_i(T_1, T_2, T_3) \cdot ON_i \rightarrow \max, \quad (1)$$

where ON_i – octane number of the i -th component according to the research method, y_i – group concentration of catalytic reforming of gasoline components.

- 2) Increasing the octane number of gasoline in reforming is achieved due to the complete conversion of naphthenic (cyclic) hydrocarbons into arenes (aromatic hydrocarbons) with a high octane number, and also due to the partial conversion of paraffins into naphthenic hydrocarbons, which in turn are converted into arenes. However, according to environmental requirements in commercial gasoline (Technical Regulation № 609 «On requirements to emissions of motor vehicles manufactured in circulation in the territory of the Russian Federation, harmful (polluting) substances», from January 1, 2016) the content of aromatic hydrocarbons and benzene in particular is limited to 35 and 1% vol. respectively. Therefore, it is necessary to set the criteria for the optimality of the benzene proportion (A_6) and the amount of aromatic hydrocarbons (A_i) in the reformat. Environmental restrictions apply to commercial gasoline and not directly to reformat. But they determine the proportion of reformat in the composition of commercial gasoline. Therefore, for catalytic reforming, this criterion value should be kept to a minimum.

$$f_2(X) = \sum_{i=6}^{11} y_{A_i}(T_1, T_2, T_3) \rightarrow \min, \quad (2)$$

$$f_3(X) = y_{A_6}(T_1, T_2, T_3) \rightarrow \min. \quad (3)$$

A decrease content of aromatic hydrocarbons and benzene in the composition in the reformat will entail a decrease in the octane number. Then, the optimality criteria (1) and (2), (3) are contradictory and can be studied in the MCO problem.

- 3) The criterion for the optimality of the catalytic reforming of gasoline is the yield of the target product – reformat. It is the product of the process minus the cracking gases. Thus, the optimality criterion is:

$$f_4(X) = 1 - \sum_{i=1}^5 y_i(T_1, T_2, T_3) - \Delta y_{H_2}(T_1, T_2, T_3) \rightarrow \max, \quad (4)$$

where Δy_{H_2} – change the proportion of hydrogen in the product. Shares can be: mass, molar, volumetric.

Based on the above optimality criteria, variable parameters and a kinetic model, the formulation of the MCO problem of conditions for catalytic reforming of gasoline based on the kinetic model is [9]:

- Vector variable parameters $X = (x_1, x_2, x_3) = (T_1, T_2, T_3)$. Where T_1, T_2, T_3 – the inlet temperature of the first, second and third reactor, respectively.
- Vector function optimality criteria $F(X) = (f_1(X), f_2(X), f_3(X), f_4(X))$. As optimality criteria for catalytic reforming considered: f_1 – RON (research octane number) (1), f_2 - content of total aromatic hydrocarbons (2), f_3 - benzene content (3), f_4 - target product reformat yield (4).

– $F(X)$ with values in target space $\{F\} = R^{(F)} = R^4$ defined in the area $D_X \subset \{X\} = R^{|X|} = R^3$: $T_1 \in [T_1^-; T_1^+]$, $T_2 \in [T_2^-; T_2^+]$, $T_3 \in [T_3^-; T_3^+]$.

Then it is necessary to maximize the optimality criteria in the D_X domain.

The mathematical model of catalytic reforming is a system of ordinary nonlinear differential equations with initial data [10].

$$\frac{dy_i}{d\tau} = \sum_{j=1}^J v_{ij}(k_j^0 \exp(-\frac{E_j^+}{RT}) \cdot \prod_{i=1}^I (\frac{y_i}{Q})^{\alpha_{ij}} - k_{-j} \cdot \prod_{i=1}^I (\frac{y_i}{Q})^{\beta_{ij}}); \quad (5)$$

$$\frac{dT}{d\tau} = -\frac{\sum_{i=1}^I \frac{dy_i}{d\tau} \cdot \Delta H_i(T)}{\sum_{i=1}^I y_i \cdot C_{pi}(T)}; \quad (6)$$

$$\frac{dQ}{d\tau} = \sum_{i=1}^I \frac{dy_i}{d\tau}; \quad (7)$$

$$\tau \in [0, \tau_1] \cup [\tau_1, \tau_2] \cup [\tau_2, \tau_3]; \quad (8)$$

$$\tau = 0 : y_i(0) = y_i^0; Q(0) = Q^0; \quad (9)$$

$$T(0) = T_1; T(\tau_1) = T_2; T(\tau_2) = T_3; i = 1, \dots, I; \quad (10)$$

$$\Delta H_i(T) = \Delta H_i(298) + \int_{298}^T C_{pi}(T) dT; \quad C_{pi}(T) = a_i + b_i T + c_i T^2 + d_i T^3 + e_i T^4; \quad (11)$$

where y_i – group concentration of reactants in reaction, mol frac.; τ – conditional contact time, kg*min/mol; J – number of stages; I – number of substances; v_{ij} – stoichiometric matrix coefficients; w_j – rate j -th stage, 1/min; k_j, k_{-j} – rate constants of forward and reverse reaction, 1/min; α_{ij} – negative matrix elements v_{ij} , β_{ij} – positive elements v_{ij} , k_j^0, k_{-j}^0 – pre-exponential factors, 1/min; E_j^+, E_j^- – activation energies of the forward and reverse reactions, kcal/mol; R – universal gas constant, kcal/mol*K); T – temperature, K, $\Delta H_i(T)$ – formation enthalpy of i -th component at a temperature T , J/mol; $C_{pi}(T)$ – specific heat capacity of the i -th component at temperature T , J/(mol*K); a_i, b_i, c_i, d_i, e_i – coefficients of the heat capacity temperature dependence i -th component; Q – molar flow rate, mol/min.

Solution (5)–(11) is a direct kinetic problem. Solution of the problem is performed by MCO algorithm Pareto approximation NSGA-II [11–13] in Matlab.

On Fig. 1 the solution to the two-criterion problem of optimizing the temperature regime in the catalytic reforming of gasoline is shown. The solution is the values of the three temperatures at the inlet of the three reactors and the corresponding values of the optimization criteria. All determined values are optimal. The choice of a specific

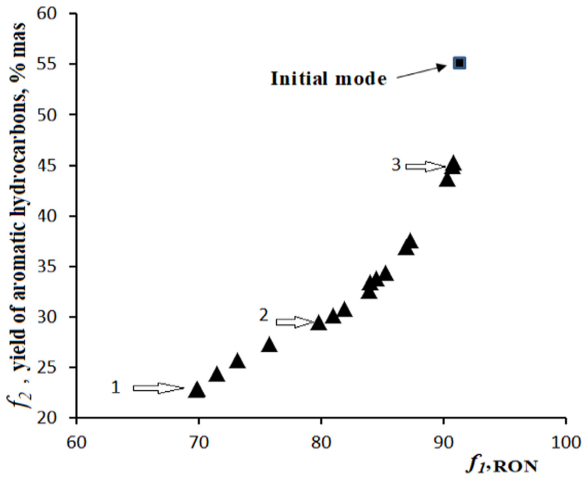


Fig. 1. Approximation of the Pareto front in MCO problem of catalytic reforming of gasoline for optimality criteria: RON, the yield of aromatic hydrocarbons.

Table 1. Approximation value set and Pareto front MCO problem for catalytic reforming of gasoline

№	$x_1 - T_1$	$x_2 - T_2$	$x_3 - T_3$	$f_1 - \text{RON}$	$f_2 - \text{Aromatic hydrocarbons, \% mass}$
1	400,0	400,0	400,0	69,8	22,8
2	499,6	426,2	440,0	81,9	30,8
3	425,6	488,0	494,7	90,7	45,0

temperature regime depends on the person making the decision. In Fig. 1, some points are marked, designated as 1, 2, 3, for which Table 1 shows the values of the varied parameters and optimality criteria. Non-improved combinations of aromatic content and RON presented in the graph in Fig. 1 represent the boundary of the range of values of possible combinations of optimality criteria (Pareto front). The physical meaning of each point is that at the current value of RON, the lowest possible aromatic content and, conversely, at the current value of aromatic, the maximum possible RON. As a result, it is possible to distinguish a mode providing a decrease in the content of the sum of aromatic hydrocarbon by 10% with a loss of RON by 2 points (point 3).

At the next stage of solving the MCO-problem for catalytic reforming of gasoline, minimization of the benzene content in the product was investigated without a significant decrease in the RON and the maximum yield of reformat (Fig. 2, Table 2).

Some highlighted points of optimal temperature regimes and the corresponding values of RON, benzene yield and reformat yield when solving the MCO problem are given in Table 2 (points 1, 2, 3 in Fig. 2). That is, each point determines three temperatures of the reaction mixture at the inlet to the reactor, providing:

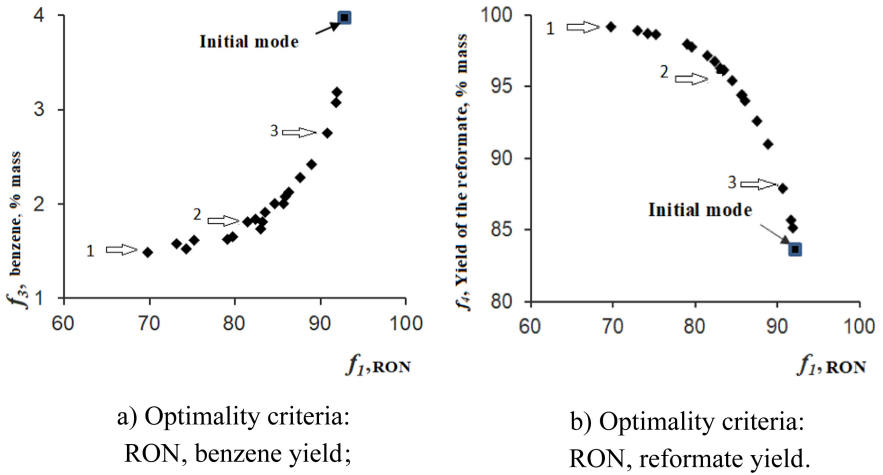


Fig. 2. Pareto front approximation of the MCO-problem for catalytic reforming of gasoline

- minimum benzene content and maximum reformate yield at the current RON,
- maximum RON value and reformate yield at the current benzene yield,
- minimum benzene and maximum RON at the current reformate yield.

It defines the physical meaning of each point on the graph of Fig. 2. The marker indicates the initial industrial mode of the process (benzene 4%; RON 92.7; reformate yield 84.3%).

Table 2. Optimal values of variable parameters and optimality criteria for the catalytic reforming of gasoline when solving MCO problem: RON, benzene yield, reformate yield

N_{Q}	$x_1 - T_1$	$x_2 - T_2$	$x_3 - T_3$	$f_1 - \text{RON}$	$f_3 - \text{yield of the benzene, \% mass}$	$f_4 - \text{yield of the reformate, \% mass}$
4	400,0	400,0	400,0	69,8	1,49	99,2
5	499,0	440,5	443,1	83,0	1,74	96,3
6	479,8	486,3	484,4	90,8	2,75	87,9

As a result, a mode was determined, in which a decrease in the content of benzene amount from 4 to 3% of the mass is achieved with a loss of RON by 1 point and an increase in the yield of reformate by 1.5% of the mass (Table 2, line 3). It is possible to distinguish the temperature regime (Table 2, line 3), at which a decrease in the benzene content from 4 to 3% of the mass is achieved, while the RON decreased from 92.7 to 91.8 points. Temperature regime No. 3 (Table 2) provides a decrease in the benzene content in the reformate by 23% with the minimum possible decrease in RON relative to the initial regime.

It should be noted that, along with the product of catalytic reforming, commercial gasoline also contains products of the catalytic cracking of vacuum gas oil and low-temperature catalytic isomerization of the pentane-hexane fraction. Therefore, a slight

decrease in RON reformat can be compensated for by the products of such processes. And the main share of aromatics and benzene in commercial gasoline belongs to the catalytic reforming reformat.

Solution of MCO problem made it possible to determine the temperature regime in reactor block, which makes it possible to reduce the benzene yield without a significant loss of octane number and with an increase in the reformat yield.

The found Pareto set is unimprovable, but in order to apply it in practice, it is necessary to study the stability of the regimes and possible areas of failure in optimal solution.

3 Mathematical Formulation of the Problem of Pareto Set Stability Analysis

Solution of the MCO problem of the conditions for carrying out the catalytic reaction (5)–(11) in the form of the Pareto frontier is denoted as $F_s^n(X)$, where X – matrix of optimal values of varied parameters $X = (x_{ij}) \in R^{s \times m}$; m – number of variable parameters, n – number of optimality criteria, s – cardinality of the set solutions to the MCO problem. Then it is necessary to analyze the stability of the Pareto frontier in the optimal conditions for carrying out catalytic processes $F_s^n(X)$ to small perturbations in the parameters based on the kinetic model.

The stable state of equilibrium of the system according to Lyapunov means that with a sufficiently small deviation from the equilibrium position, the system will never go far from the singular point [14]. Pareto frontier $F_s^n(X)$ is stable in the case when, for small independent perturbations of the matrix elements X set values s - effective trajectories deviate from the initial state by some small values.

By analogy with [14], the definition of the stability of the Pareto frontier $F_s^n(X)$: if $B = (b_i) \in R^m$ – disturbance vector to X , can always find a vector $\Delta = (\delta_j) \in R^n$.

$$\forall b_i > 0 \exists \Delta : |F_s^j(X) - F_s^j(X + B)| \leq \delta_j, \quad (12)$$

where $i = 1, \dots, m$; $j = 1, \dots, n$.

Then the radius of stability of the Pareto frontier defined as

$$\rho_s^j(X) = \begin{cases} \sup P_j(X), & \text{if } P(X) \neq \emptyset \\ 0, & \text{if } P(X) = \emptyset \end{cases}, \quad (13)$$

where $P_j(X) = \{B > 0 \mid |T_s^j(X) - T_s^j(X + B)| \leq \delta_j\}$.

The Pareto frontier of the problem $F_s^n(X)$ is stable if and only if $\rho_s^j(X) > 0$, $j = 1, \dots, n$ [1]. Moreover, depending on the set of permissible deviations Δ , different radius of stability is determined by variable parameters.

Thus, it is proposed to evaluate the influence of the disturbance of optimal values of all investigated variable parameters on the values of optimality criteria.

4 Parallel Algorithm for Analyzing the Stability of the Pareto Frontier

According to the definition of stability Pareto frontier for the conditions for carrying out catalytic reactions based on the kinetic model (1)–(11), an algorithm for calculating the radius of stability of the problem is developed in this work (Fig. 3).

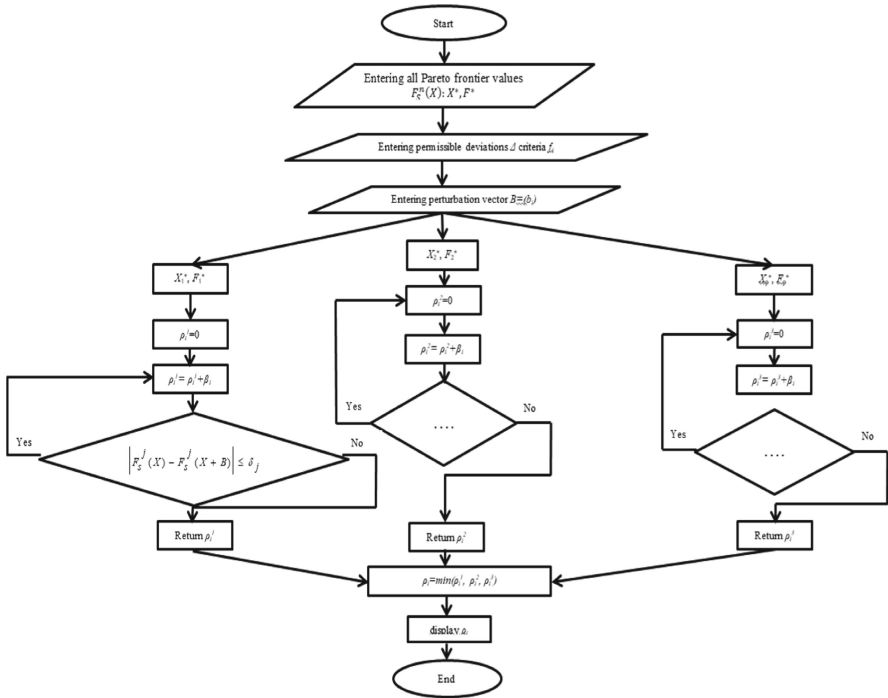


Fig. 3. Block diagram of a parallel algorithm for calculating the stability radius of the MCO solution

Input data are: calculated values of the Pareto frontier $F_s^n(X)$ – matrix of optimal values for varied parameters X^* , values optimality criteria F^* , values of permissible deviations Δ optimality criteria f_j , disturbance vector B for each optimality criterion. The stability radius is determined for each variable parameter based on the definition of the stability of the Pareto frontier (12).

According to Fig. 2 the parallelization is realized by elements of the Pareto sets X^* , F^* . Depending on the number of available processors P sets X^* , F^* are divided into P subsets.

$$X^* = \bigcup_{p=1}^P X_p^*,$$

$$F^* = \bigcup_{p=1}^P F_p^*.$$

On subsets of elements in Pareto set, the stability radius of each variable parameter is calculated ρ_i^p . Next, the calculated ρ_i^p returned to the main process and for each of them varied parameter is selected the smallest of the calculated values.

5 Research Results

For the catalytic reforming of gasoline solution MCO conditions of the catalytic reaction (1), (2) Pareto frontier is denoted as $F_s^n(X)$. $m = 3$ – number of variable parameters, $n = 4$ – number of optimality criteria, $s = 50$ – cardinality of the set solutions to the MCO problem. Then it is necessary to analyze the stability of the Pareto frontier of the optimal conditions for carrying out catalytic processes $F_{50}^4(X)$ to small perturbations in the parameters based on the kinetic model [15, 16].

For the process of catalytic reforming of gasoline, the stability radius were calculated for three temperatures at the inlet to the reactor of the unit.

In determining the values of acceptable change calculated trajectories Δ assume no more than 2% octane. Not more than 10% in aromatics yield, 10% in benzene yield, 10% in reformat yield.

$$\Delta = (\delta_1, \delta_2) = (0.02, 0.1, 0.1, 0.1, 0.1). \quad (14)$$

Perturbations are set for variable parameters - three temperatures at the inlet to the block reactor: $B = (b_1, b_2, b_3)$. The stability radius is determined for each variable parameter, according to the algorithm in Fig. 2. The calculated permissible temperature change at the inlet to the reactor blocks corresponding to the permissible changes in the values of the optimality criteria (14) is 22 °C.

Consecutive calculation for all elements of the Pareto set takes considerable time, due to the complexity of solving the direct kinetic problem (5) - (11). Therefore, the parallelization of the computational process was implemented by the elements of the calculated Pareto set, according to the algorithm in Fig. 2.

The computational experiment time depending on the number of processors is shown in Fig. 3. For the calculation, use a 4-core PC Intel Core i7-8550U CPU, RAM 16GB, OS Windows10, Software system: Matlab (MATrix LABoratore).

To assess parallelization acceleration and efficiency was defined (Fig. 4). For the selected algorithm parallelizing of computational process stability radius calculation for catalytic reforming solutions MCO problem gasoline efficiency is 74% (Fig. 5).

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

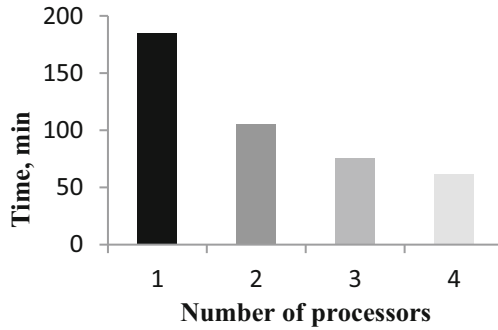


Fig. 4. Computing experiment time depending on the number of processors

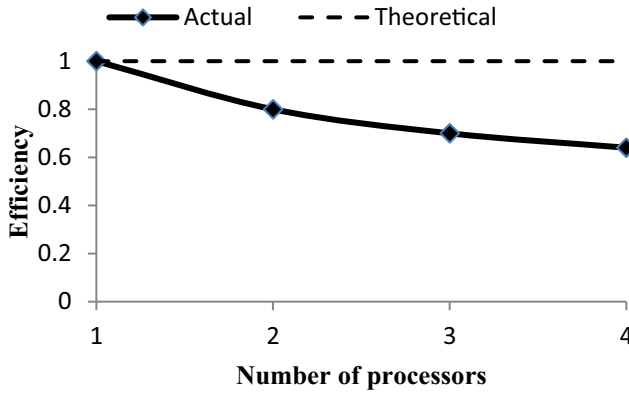


Fig. 5. Efficiency of the parallel program for calculating the stability radius of the MCO problem solution

6 Conclusion

The multicriteria optimization for the conditions for multistage chemical reactions based on the kinetic model is relevant for both laboratory and industrial processes. Complex multistage chemical processes require the determination of the permissible ranges for parameter values that ensure the stability of the calculated solution with an acceptable error, for the application of the obtained solutions in practice. In the catalytic reforming of gasoline MCO conditions solved the problem based on a kinetic model and calculated optimal radius resistance values of the inlet temperature to the reactor. Calculated allowable change in temperature at the inlet of reactor blocks corresponding to changes in allowable values optimality criteria (12) is 22 °C. A parallel algorithm for solving the problem of analyzing the stability of the Pareto set is developed and the efficiency of parallel program execution is estimated. The defined efficiency of the developed parallelization algorithm for calculating the stability radius of the solution to the MCO problem was 74%. The developed parallel algorithm for calculating the

stability of the Pareto frontier will be used to analyze other catalytic industrial and laboratory processes [17, 18].

Acknowledgement. This research was performed due to the Russian Science Foundation grant (project No. 21-71-20047).

References

1. Bukhtoyarov, S.E., Emelichev, V.A.: Parametrization of the optimality principle (“from Pareto to Slater”) and stability of multicriteria trajectory problems. *Disc. Anal. Oper. Res.* **10**(2), 3–18 (2003)
2. Akhmadiev, F.G., Gizzyatov, R.F., Nazipov, I.T.: Mathematical modeling of kinetics and optimization of grain material separation processes on sieve classifiers. *Lobachevskii J. Math.* **41**(7), 1155–1161 (2020)
3. Gubaidullin, D.A., Snigerev, B.A.: Mathematical modelling of gas flow with heavy solid particles based on eulerian approach. *Lobachevskii J. Math.* **40**(11), 1944–1949 (2019)
4. Podgaets, A.R.; Ockels, W.J.: Stability of optimal solutions: multi- and single-objective approaches. In: *IEEE Symposium on Computational Intelligence in Multi-Criteria Decision-Making*, pp. 395–402 (2007)
5. Gitman, M.B., Trusov, P.V., Yakubovich, M.B.: Stability of contracted beam with stochastic distribution of initial parameters. In: *Proceedings of XIII School on Simulations in Continuous Medium Mechanics*, pp. 152–159 (1999)
6. Emelichev, V., Kuz'min, K., Nikulin, Y.: Stability analysis of the Pareto optimal solutions for some vector boolean optimization problem. *Optimization* **54**(6), 545–561 (2005)
7. Zagoruiko, A.N., Noskov, A.S., Belyi, A.S., Smolikov, M.D.: Unsteady-state kinetic simulation of naphtha reforming and coke combustion processes in the fixed and moving catalyst beds. *Catal. Today* **220**, 168–177 (2014)
8. Zainullin, R.Z., Zagoruiko, A.N., Koledina, K.F., Gubaidullin, I.M., Faskhutdinova, R.I.: Multi-criterion optimization of a catalytic reforming reactor unit using a genetic algorithm. *Catal. Ind.* **12**(2), 133–140 (2020). <https://doi.org/10.1134/S2070050420020129>
9. Koledina, K.F., Koledin, S.N., Karpenko, A.P., Gubaydullin, I.M., Vovdenko, M.K.: Multi-objective optimization of chemical reaction conditions based on a kinetic model. *J. Math. Chem.* **57**(2), 484–493 (2018). <https://doi.org/10.1007/s10910-018-0960-z>
10. Zainullin, R.Z., Koledina, K.F., Akhmetov, A.F., Gubaidullin, I.M.: Kinetics of the catalytic reforming of gasoline. *Kinet. Catal.* **58**(3), 279–289 (2017)
11. Deb, K., Mohan, M., Mishra, S.: Towards a quick computation of well-spread Pareto-optimal solutions. In: Fonseca, C.M., Fleming, P.J., Zitzler, E., Thiele, L., Deb, K. (eds.) *EMO 2003. LNCS*, vol. 2632, pp. 222–236. Springer, Heidelberg (2003). https://doi.org/10.1007/3-540-36970-8_16
12. Srinivas, N., Deb, K.: Multiobjective optimization using nondominated sorting in genetic algorithms. *Evol. Comput.* **2**(3), 221–248 (1994)
13. Munoz, M.A., Kirley, M., Halgamuge, S.K.: Exploratory landscape analysis of continuous space optimization problems using information content. *IEEE Trans. Evol. Comput.* **19**(1), 74–87 (2015)
14. Emelichev, V.A., Girlich, E., Nikulin, Y., Podkopaev, D.P.: Stability and regularization of vector problems of integer linear programming. *Optimization* **51**(4), 645–676 (2002)

15. Koledina, K.F., Koledin, S.N., Nurislamova, L.F., Gubaydullin, I.M.: Internal parallelism of multi-objective optimization and optimal control based on a compact kinetic model for the catalytic reaction of dimethyl carbonate with alcohols. In: Sokolinsky, L., Zymbler, M. (eds.) PCT 2019. CCIS, vol. 1063, pp. 242–255. Springer, Cham (2019). https://doi.org/10.1007/978-3-030-28163-2_17
16. Lotov, A.V., Ryabikov, A.I.: Launch pad method in multiextremal problems of multicriteria optimization. *J. Comput. Math. Math. Phys.* **59**(12), 2111–2128 (2019)
17. Vovdenko, M.K., Gabitov, S.A., Koledina, K.F., Ahmerov, E.A., Sannikov, A.D.: Mathematical modeling of isopropylbenzene oxidation reaction and oxidation reactor. *IOP Conf. Ser. J. Phys. Conf. Ser.* **1096**, 012189 (2019)
18. Koledina, K.F., Gubaidullin, I.M., Koledin, S.N., Baiguzina, A.R., Gallyamova, L.I., Khusnutdinov, R.I.: Kinetics and mechanism of the synthesis of benzylbutyl ether in the presence of copper-containing catalysts. *Russ. J. Phys. Chem. A* **93**(11), 2146–2151 (2019). <https://doi.org/10.1134/S0036024419110141>