SCIENTIFIC CONFERENCE

Russian Supercomputing Days

Parallel algorithm for calculating the radius of stability in multicriteria optimization conditions for catalytic reforming of gasoline

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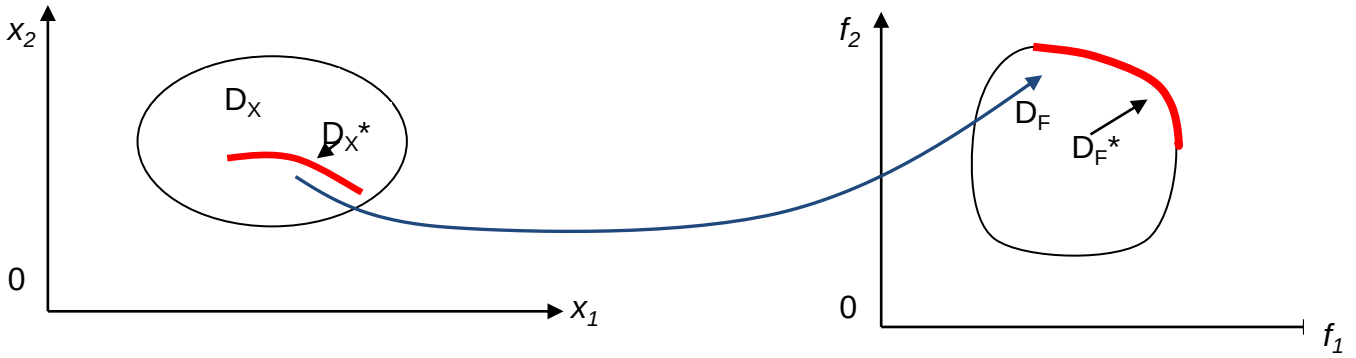
The task of multicriteria optimization

X - vector of variable parameters ; D_X - the set of admissible values of the vector X; $F(X)=(f_1(X), f_2(X),\ldots, f_{|F|}(X),)$ – vector function of optimality criteria ; $F(X)$ displays a set D_X in a set $\boldsymbol{D_F}$ **– set of reachability.**

Subset $D_F^* \subset D_F$ - **Pareto front values (optimality criteria)**. Subset $\boldsymbol{D_X^*} \subset D_X$ - Pareto set values (variable parameters) .



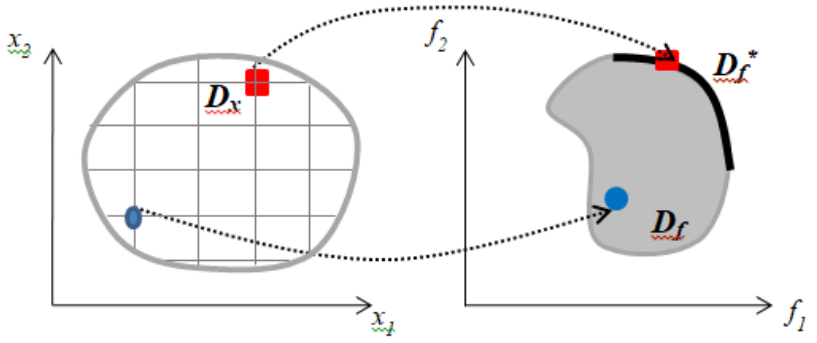
- **Vallerio M, Telen D, Cabianca L, Impe J Van, Logist F, Manenti F (2016) Robust multi-objective dynamic optimization of chemical processes using the Sigma Point method. Chem Eng Sci 140:81-89**
- **Sun X, Kim S, Yang SD., Kim HS, Yoon JY (2017) Multi-objective optimization of a Stairmand cyclone separator using response surface methodology and computational fluid dynamics. Powder Technol 320:51–65**
- **Koledina KF, Koledin SN, Karpenko AP, Gubaydullin IM, Vovdenko MK (2019) Multi-objective optimization of chemical reaction conditions based on a kinetic model. J Math Chem 57(2):484–493**

Algorithms for solving the MCO problem

A priori algorithms

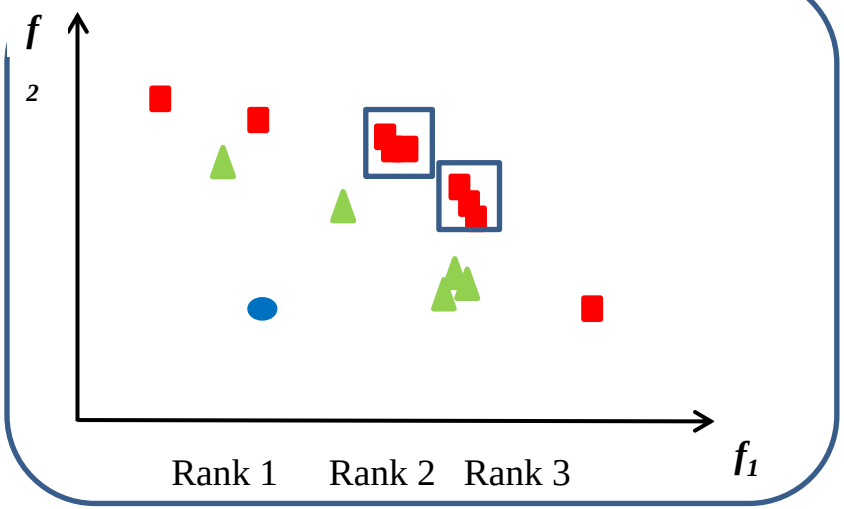
$$F(X) = \sum_{l=1}^{|F|} \lambda_l f_l(X),$$

Grid Algorithm

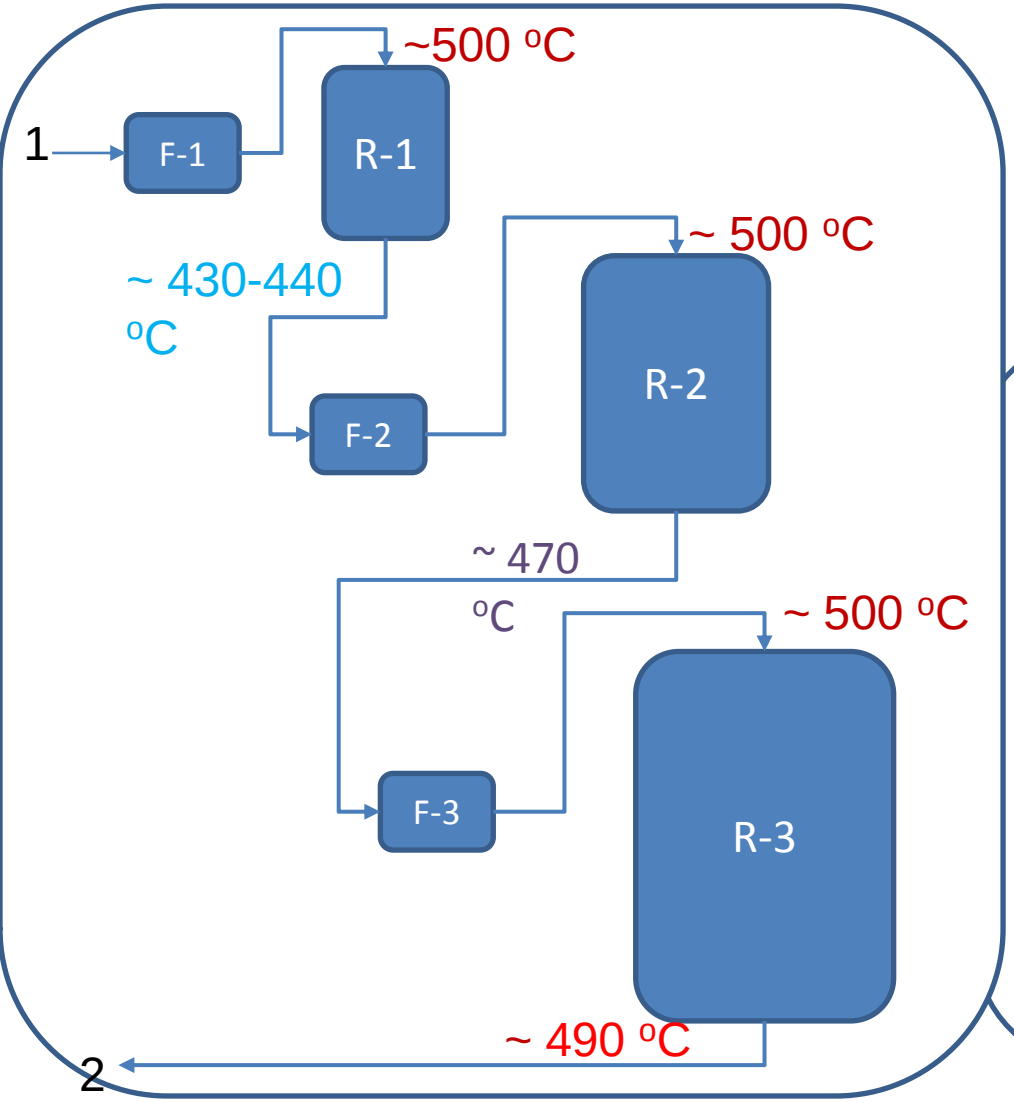


NSGA-II*

- **Kalyanmoy Deb. Multi-Objective optimization using evolutionary algorithms. India. 2001.**
- **A.P. Karpenko. Modern search engine optimization algorithms. Publishing house of MSTU im. N.E. Bauman. 2014**



Experimental data on gasoline catalytic reforming



Unit L-35-11/300

Bimetallic alumina-base catalyst RG-682 (platinic-rhenium) - Pt-Re/Al_2O_3

F-1,2,3 – furnaces for further heating,

R-1,2,3 – reactors

Table. Techological mode of the reactor section

Criteria	Values
Inlet temperature at R-1°C	489,0
Outlet temperature at R-1, °C	422,0
Inlet temperature at R-2, °C	489,0
Outlet temperature at R-2, °C	457,0
Inlet temperature at R-3, °C	489,0
Outlet temperature at R-3, °C	474,0
Inlet pressure at R-1, kgf/cm²	23,0
Water supply, liters per day:	4,5
Chlorum supply, liters of dichloroethane per day:	1,1
Recycled gas usage, Nm³/hr:	66500,0

Mathematical description of non-isothermal reaction of gasoline catalytic reforming accounting molecule number changes can be written down as (1)-(6)

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

$$\frac{dM}{d\tau} = \sum_{i=1}^{I} \frac{dy_i}{d\tau}; \quad (2)$$

$$\frac{dT}{d\tau} = -\frac{\sum_{i=1}^{I} \frac{dy_i}{d\tau} \cdot \Delta H_i(T)}{\sum_{i=1}^{I} y_i \cdot C_{pi}(T)}; \quad (3)$$

$$\tau \in [0, \tau_1] \cup [\tau_1, \tau_2] \cup [\tau_2, \tau_3]; \quad (4)$$

$\tau=0$: $y_i(0)=y_i^0$; $Q(0)=Q^0$;
$T(0)=T_1$; $T(\tau_1)=T_2$; $T(\tau_2)=T_3$; $\quad i = 1,\ldots I$; (5)

$$\Delta H_i(T) = \Delta H_i(298) + \int_{298}^{T} C_{pi}(T)dT; \quad C_{pi}(T) = a_i + b_i T + c_i T^2 + d_i T^3 + e_i T^4. \quad (6)$$

y_i – concentration of substances, mol. frac.;
τ – contact time, kg*h/mol;
M – changing the number of moles in the reaction mixture (mol / min);

Optimization of conditions of gasoline catalytic reforming

Variable parameters

$x_1 = T_1 \in [400\ ;500\ ]$

$x_2 = T_2 \in [400\ ;500\ ]$

$x_3 = T_3 \in [400\ ;500\ ]$

To resolve this multi criteria optimization task, the authors used the Pareto approximation algorithm NSGA-II.

Optimality criteria

- **Octane number** (additivity of the octane number)

$$f_1(X) = ONRM\ \ (T_1, T_2, T_3) = \sum_{i=1}^{I} y_i(T_1, T_2, T_3) \cdot ONRM_{\ i} \rightarrow \max$$

- **Content of aromatic hydrocarbons and benzol should be minimized for catalytic reforming**

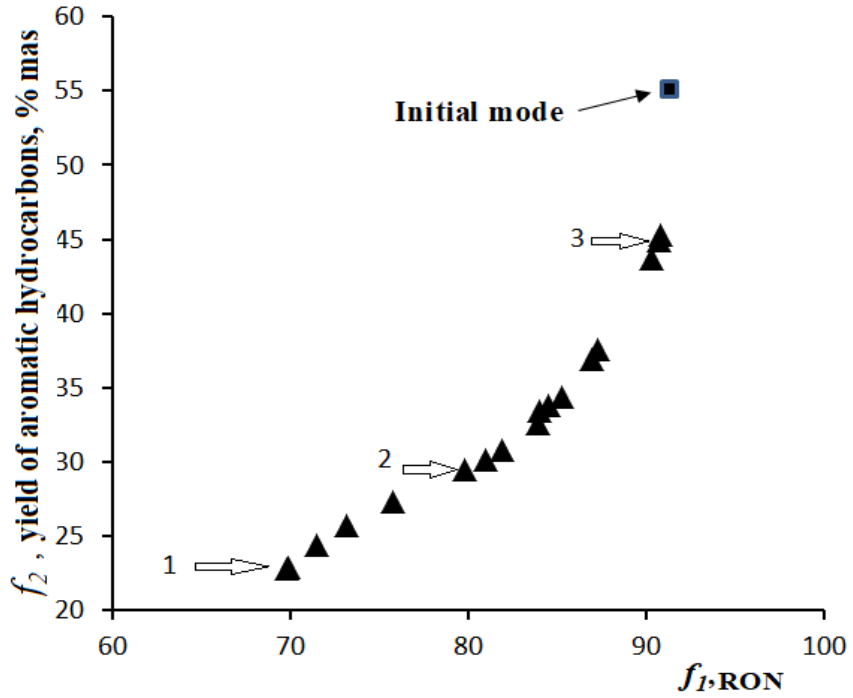
$$f_2(X) = \sum_{i-6}^{11} y_{A_i}(T_1, T_2, T_3) \rightarrow \min \qquad f_3(X) = y_{A_6}(T_1, T_2, T_3) \rightarrow \min$$

- **Yield of the target product — reformate**

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

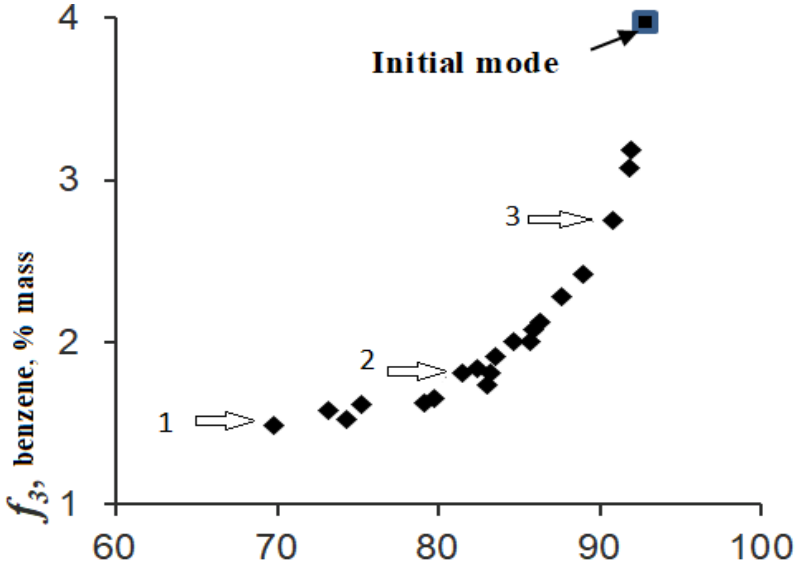
$$\max_{X \in D_X} F(X) = F(X^*) = F^*.$$

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

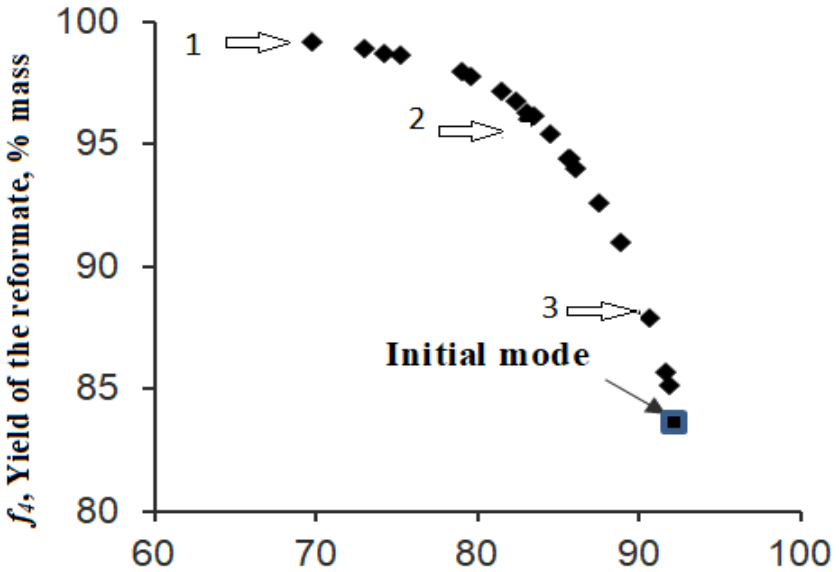


№	x_1 - T_1	x_2 - T_2	x_3 - T_3	f_1 -RON	f_2 - Aromatic hydrocarbons, % mass
1	400,0	400,0	400,0	69,8	22,8
2	499,6	426,2	440,0	81,9	30,8
3	425,6	488,0	494,7	90,7	45,0

Optimal values of variable parameters and optimality criteria for the catalytic reforming of gasoline : RON, benzene yield, reformate yield



a) Optimality criteria: $f_{1,\mathrm{RON}}$
RON, benzene yield



b) Optimality criteria: $f_{1,\mathrm{RON}}$
RON, reformate yield.

№	$x_1 - T_1$	$x_2 - T_2$	$x_3 - T_3$	f_1 – RON	f_3 – yield of the benzene, % mass	f_4 – yield of the reformate, % mass
1	400,0	400,0	400,0	69,8	1,49	99,2
2	499,0	440,5	443,1	83,0	1,74	96,3
3	479,8	486,3	484,4	90,8	2,75	87,9

Mathematical formulation of the problem of Pareto set stability analysis

$F_s^n(X)$ - solution of the MCO problem of the conditions for carrying out the catalytic reaction in the form of the Pareto frontier

X – matrix of optimal values of varied parameters $X = (x_{ij}) \in R^{s \times m}$

$B = (b_i) \in R^m$ – disturbance vector to X, can always find a vector $\Delta = (\delta_j) \in R^n$

$$\forall b_i > 0 \; \exists \Delta : \left| F_s^j(X) - F_s^j(X + B) \right| \leq \delta_j$$

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

Then the radius of stability of the Pareto frontier defined as

$$\rho_s^j(X) = \begin{cases} supP_j(X), \text{ if } P(X) \neq \varnothing \\ 0, \text{ if } P(X) = \varnothing \end{cases}$$

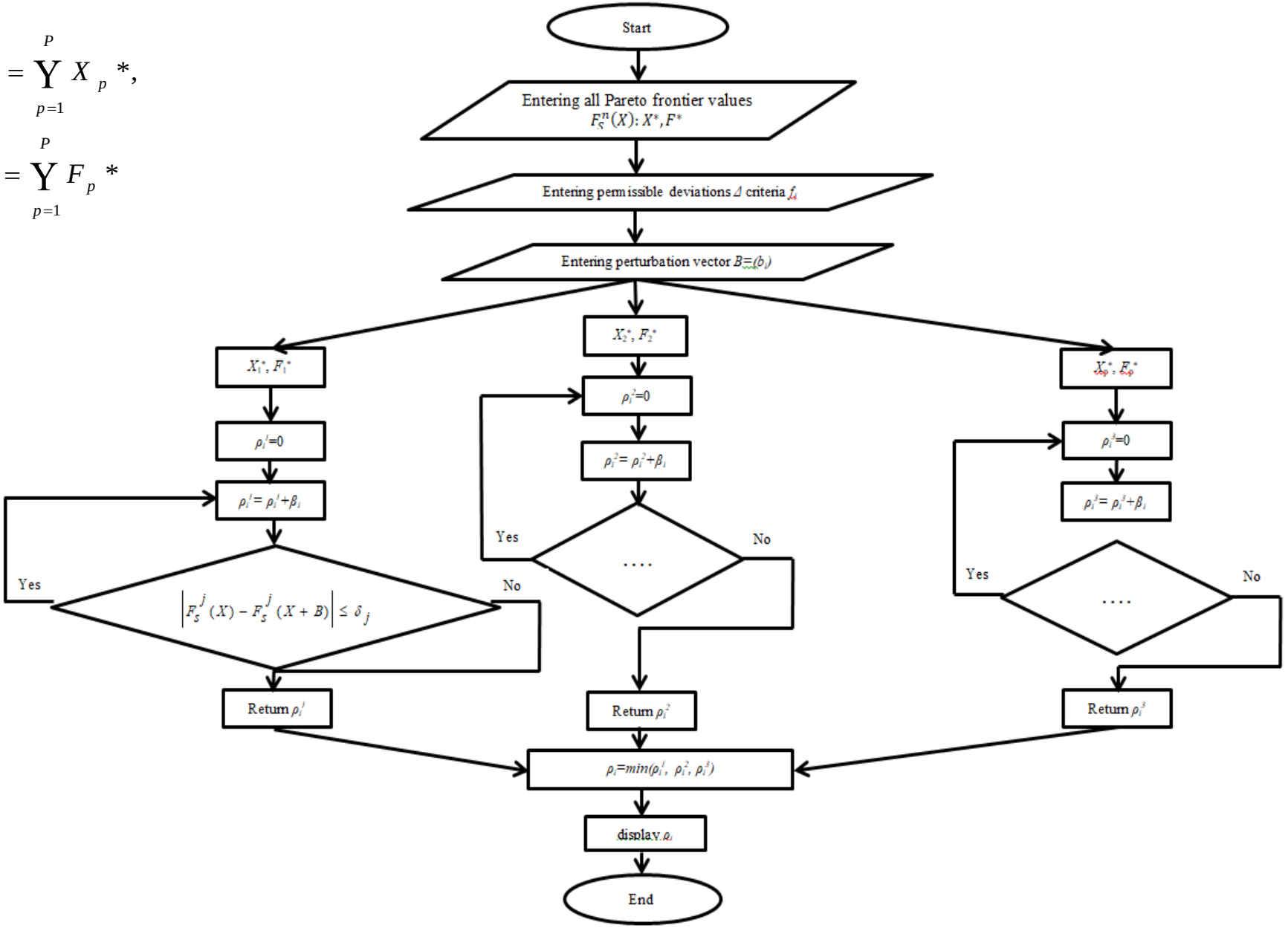
where $P_j(X) = \{B > 0 \mid \left| T_s^j(X) - T_s^j(X + B) \right| \leq \delta_j\}$

The Pareto frontier of the problem $F_s^n(X)$ is stable if and only if $\rho_s^j(X) > 0$, $j=1,...,n$

Parallel algorithm for analyzing the stability of the Pareto frontier

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

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



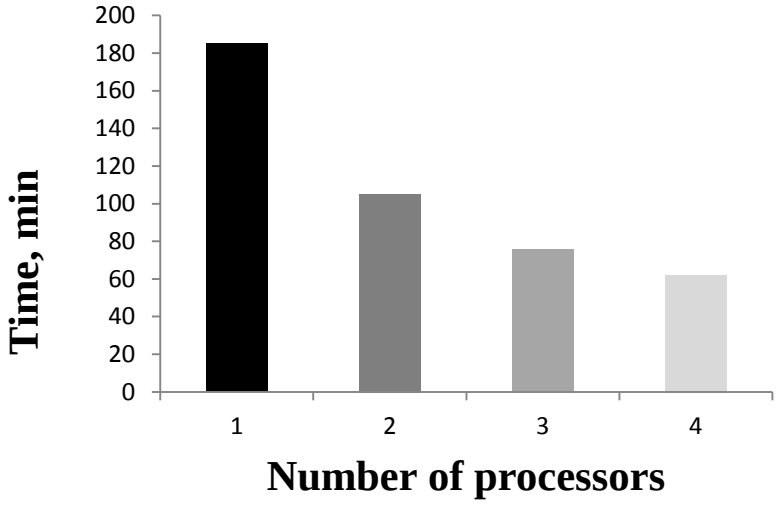
Research results

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 reformate yield.

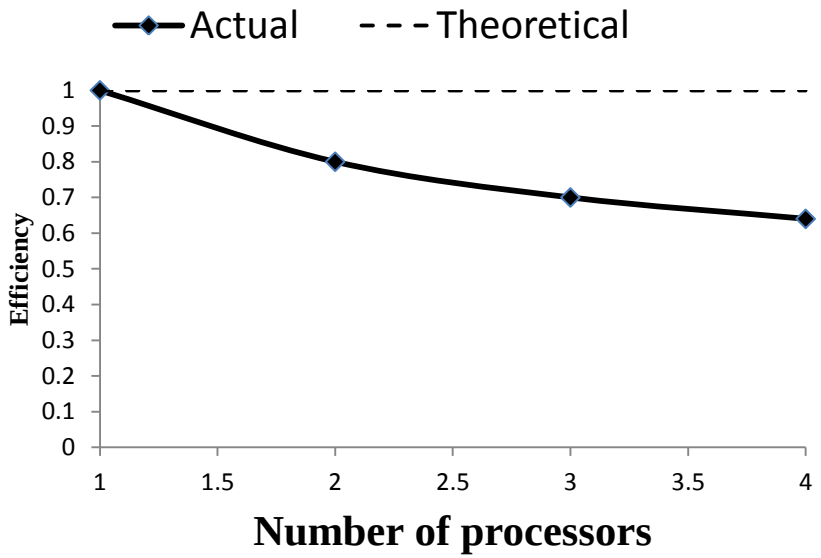
$$\Delta = (\delta_1, \delta_2) = (0.02, 0.1, 0.1, 0.1).$$

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 is 22°C.

Research results



Computing experiment time depending on the number of processors



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

Conclusion

- 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%.

Thank you for attention!