UDC 66.023.2

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TO CALCULATION OF OPTIMIZATION PROBLEM OF THE CHEMICAL PROCESS IN ISOTHERMIC REACTOR IDEAL REMOVAL

Abstract: *In article, it was dealed with the model of ideal mixing and idealized flow entering the reactor which instantly distributed throughout the volume as a result of the complete (ideal) mixing of the medium particles. It was used the half-division method (dichotomy method) of the intervals in the MathCAd medium. It was used the system of algebraic equations of material and thermal equilibrium. We have determined the optimal concentration of the components of the reaction in the stationary mode,*

Optimization of the problem of the output of the target product for the isothermal thermal regime and the chemical process gave the possibility to obtain the maximum value of the function at given points and to calculate the residence time of the substances in the reaction at each reaction interval depending on the change of the concentration of the reactant substance for the chosen chemical process and the given coefficients.

Keywords**:** *ideal mixing model, concentration, half-division method (dichotomy method*).

INTRODUCTION, PROBLEM STATEMENT

In chemical technology, the approach to the ideal mixing is achieved by installing special mixers in machines [1, 2]. Many chemical processes are close to the ideal mixing mode, and therefore in such reactors, theoretically, instantaneous and complete mixing of substances entering the apparatus is provided. Then, in many cases, processes can be described with an approximation sufficient for practice in the ideal mixing model. [1, 3, 5, 7].By applying intensive mixing it is possible to achieve such a state, when the concentration of matter at all points of the reactor volume becomes practically the same[4,5-9].

LITERARY ANALYSIS

Summarizing the arguments of many researchers [4,6,7], it can be argued that the ideal mixing model is an idealized flow and is a theoretical model. According to this model, it is assumed that the stream entering the reactor is instantly distributed throughout the volume as a result of the complete (ideal) mixing of the medium

particles in [1,2,3,10]. In this case, the concentration of the distributed matter at all points of the reactor and in the output stream is the same [12,14,16].

MAIN ARTICLE

The task of optimizing the operation of the reactor belongs to the simplest optimization problems[2,3,6]. The criterion for optimality of this problem is the function of one variable. Thus, optimizing the output of the target component in an isothermal reactor of a perfect mixing means finding a function of the time of its stay [2,3].

In this case, the concentration of components at the exit from the reactor is equal to the concentration in the reaction zone. In the general case, stationary mode is described by a system of algebraic equations of material and thermal equilibrium for each component [8, 12]:

$$\begin{cases} \frac{1}{\tau}(C_{exi} - C_i) + W_i = 0; \\ \frac{1}{\tau}(T_{exi} - T) + \frac{1}{C}(\pm\Delta H)|W_i| - \frac{K \cdot F}{C_x \cdot V_x}(T - T_x) = 0; \\ \frac{1}{\tau}(T_{exi} - T) + \frac{K \cdot F}{C_x \cdot V_x}(T - T_x) = 0; \end{cases} \quad \textbf{(1)}$$

n - the number of components of the reaction; *x* - average time of stay of a stream in the reactor; *Cvh*i, *Ci* - input, current (initial) concentration of i-th component; *T*, *Tx* - input, current (output) flow temperature, respectively; *Cx* - volumetric heat capacity*; W* - working volume of reactor and shirt; *F* - coefficient and heat transfer surface; *Vx* is the rate of conversion of the i-th component in the chemical reaction; *H* - total thermal effect; *Vx* is the total reaction rate for all stages.

Method of solution. The solution of the problem of optimizing the output of components in such a reactor is often based on solving multidimensional optimization problems[2,3]. A convenient one-dimensional method for optimizing the problems of chemical technology is the method of dichotomy using quadratic approximation[15,16].

Solution. Consider a flow reactor with a stirrer, whose mode with sufficient approximation meets the conditions of perfect mixing [14].

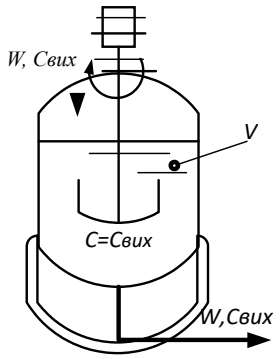

Fig. 1. *Model of perfect mixing [14]*

The complex chemical reaction is inthe reactor. That is the method of dichotomy with the help of the method of half-division of intervals.We optimize the maximum possible concentration of the half-product, which is the target component and corresponds to the time of the flow of the stream. Consequently, the criterion of optimality is the concentration of substances, and the variable - the time of stay. By the half-division method, we make the minimum number of calculations according to the model for finding. Thus, the static model of the ideal mixing reactor is given in [1, 2 ,3, 8]. In a static isothermal mode, the process of perfect mixing can be described by the equation of the material balance:

$$C_{вх}\text{-}C_i+W_{ri}=0. \quad \textbf{(2)}$$

Known concentrations of components in the inlet flow: kmol/m^3; ; $C_{рвх}=C_{Sвх}=0$. Constant speeds of individual stages of the reaction: $k_1=0{,}5h^{-1}$; $k_2=0{,}4h^{-1}$; t-time of the flow of the reactor. We have a chemical reaction like: $A \overset{k1}{\rightarrow} R \overset{k2}{\rightarrow} S$.

Total velocity of costs and formation of components in the considered reaction, that is kinetic model:

$$\begin{cases} Wr_A = \frac{dC_A}{dt} = -k_1 C_A \\ Wr_R = \frac{dC_B}{dt} = k_1 C_A - k_2 C_R \\ Wr_S = \frac{dC_S}{dt} = k_2 C_R \end{cases} \quad \textbf{(3)}$$

Mathematical model in statics:

$$\begin{gathered} \frac{1}{\tau}(\boldsymbol{C_{A0} - C_A}) - \boldsymbol{k_1 C_A} = \boldsymbol{0} \\ \frac{1}{\tau}(\boldsymbol{C_{R0} - C_R}) + \boldsymbol{k_1 C_A - k_2 C_R} \\ \frac{1}{\tau}(\boldsymbol{C_{S0} - C_S}) + \boldsymbol{k_2 C_R} = \boldsymbol{0} \end{gathered} \quad \textbf{(4)}$$

Reordering, we get:

$$C_{A0} = (1 + k_1\tau)C_A$$
$$C_{R0} = -k_1\tau C_A + k_2\tau C_R \quad \textbf{(5)}$$
$$C_{S0} = (1 - k_2\tau)C_R$$

Matrix of coefficients: C = K · C, where C, S_{vh} - vector of columns of input and output concentrations of components, respectively:

$$C=\begin{Vmatrix} C_A \\ C_R \\ C_S \end{Vmatrix} C_{вх}=\begin{Vmatrix} C_{Aвх} \\ C_{Rвх} \\ C_{Sвх} \end{Vmatrix} K = \begin{Vmatrix} 1+k_1\tau & 0 & 0 & 0 \\ -k_1\tau & k_2\tau & 0 & 0 \\ 0 & 0 & 1-k_2\tau & 1 \end{Vmatrix} \quad \textbf{(6)}$$

After the inversion of the quadratic matrix of coefficients, we have a final solution: $C=K^{-1}\cdot C_{вх}$

Next, for graphical optimization of this problem, assume that the optimized function has one maximum. We break the interval into two equal subintervals, each of which is divided into two equal parts. We calculate the value of the optimality criterion at the boundaries of all sub-intervals, including the endpoints[10,11].

Among the obtained values, we find the most, which corresponds to the type of maximum extremum [15].

$$k_2(tem) := 1{,}93 \cdot 10^8 \cdot e^{\frac{-58100}{8.31 \cdot tem}} p := 810,$$
$$i := 1..5, t_0 := 0, \Delta t := 0{,}1, C_{Ao} := 1.15,$$

Cs =

	0
0	0
1	$1.838 \cdot 10^{-5}$
2	$4.887 \cdot 10^{-5}$
3	$9.137 \cdot 10^{-5}$
4	$1.458 \cdot 10^{-4}$

Cr =

	0
0	0.01
1	0.017
2	0.023
3	0.03
4	0.036

Ca =

	0
0	1.15
1	1.143
2	1.137
3	1.13
4	1.124

Δ =

	0
0	0
1	0.066
2	0.065
3	0.065
4	0.065

t =

	0
0	0
1	0.1
2	0.2
3	0.3
4	0.4

Cs =

	0
0	0
1	$1.838 \cdot 10^{-5}$
2	$4.887 \cdot 10^{-5}$
3	$9.137 \cdot 10^{-5}$
4	$1.458 \cdot 10^{-4}$

$$C_{Ro} := 0.01,\ C_{So} := 0, F := 2.1, T_0 := 0\ , T_K := 393, k_1(tem)$$
$$:= 1{,}84 \cdot 10^9 \cdot e^{\frac{-60910}{8.31 \cdot tem}}$$

Fig.2. *Output data in MathCAD [15]: k - reaction rate constants, 1 / c, Δt - value of the integration step, T - temperature, K at the initial time, i - integration steps, Q - thermal effect of the reaction on substance S, J/kmol, c - specific heat of the reaction mixture , J/(kg · K), ρ - density of reaction mixture, kg / m3, V - volume of reaction mixture, m^3, F - surface of heat transfer, m^2, k - heat transfer coefficient, W / m^2, Tt = 383 K - coolant temperature, K, c- concentration of substances, kmol/m^3*

System of differential equations:

$$\begin{aligned} \mathrm{FC}_A(\mathrm{C}_A, tem) &:= -k_1(tem) \cdot C_A \\ \mathrm{FC}_R(\mathrm{C}_A, \mathrm{C}_R\ tem) &:= k_1(tem) \cdot C_A - k_2(tem) \cdot C_R \\ \mathrm{FC}_s(\mathrm{C}_s, tem) &:= k_2(tem) \cdot C_R \end{aligned} \quad \textbf{(7)}$$

Implementation of the Euler method and the method of dichotomy[15]:

$$\begin{pmatrix} t_i \\ C_{Ai} \\ C_{Ri} \\ C_{Si} \end{pmatrix} := \begin{pmatrix} t_{i-1} + \Delta t \\ \mathrm{C}_{Ai-1} + FC_A(\mathrm{C}_{Ai-1}, tem_0) \cdot \Delta t \\ \mathrm{C}_{Ri-1} + FC_R(\mathrm{C}_{Ai-1}, \mathrm{C}_{Ri-1}, tem_0) \cdot \Delta t \\ \mathrm{C}_{Si-1} + FC_S(\mathrm{C}_{Ri-1}, tem_0) \cdot \Delta t \end{pmatrix} \Delta_i := |FC_A(\mathrm{C}_{Ai}, tem_0)| \quad \textbf{(8)}$$

We obtain for constructing a static mathematical model of the perfect mixing matrix of coefficients K for five values of the time of stay and using MathCaD, get a graph.

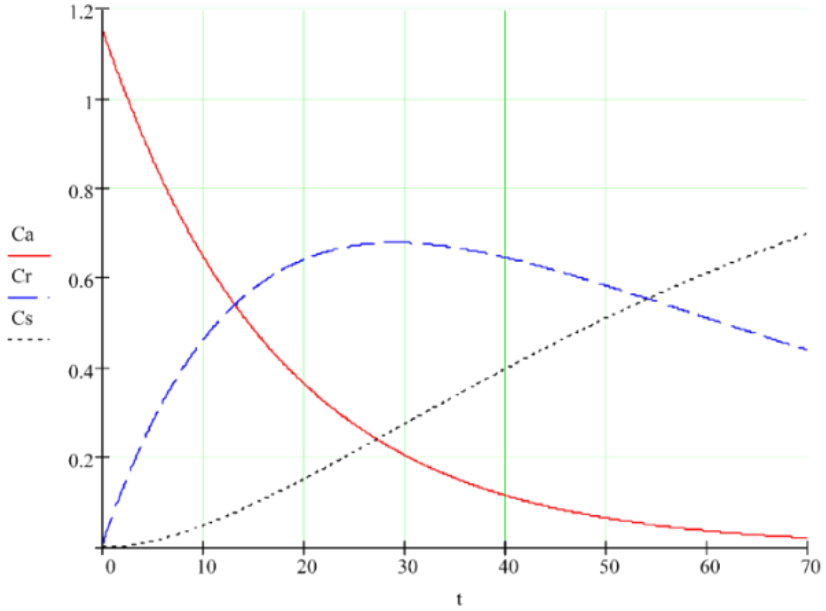

Fig.3. *Dependence of the concentration of the chemical reaction on the residence time of the substance in the reactor of perfect mixing [15]*

As we see from Fig. 2, concestration in modeling the perfect mixing process for the selected parameters k1, k2 varies proportionately. The residence time increases with the decrease in the concentration of the input substances. At the final stage, for this isothermal thermal regime, the concentration of matter and time varies parabolic

To calculate a new interval, we repeatedly repeat the procedure up to five times, until the accuracy between the values at neighboring points becomes less

than the given accuracy of the extremum. Similarly, we find the minimum of functions.

CONCLUSIONS

Using the numerical method of optimizing the half-division of intervals and mathematical programs of MathCad, we determined the optimum of the function of a variable inside a given interval by reducing the search interval for a given chemical process. Also, we determined the optimal concentration of reaction components in steady state through a system of algebraic equations of material and thermal equilibrium.

The optimization of the output of the target product for the isothermal thermal regime and the chemical process is that we used the most effective method of direct search, namely, the method of half-division of intervals in the environment of MathCad. The maximum value of a function at given points is possible using direct calculations or simulation experiments.

Consequently, the mathematical description for isothermal thermal regime is solved by dichotomy with a constant integration step and allows to calculate the residence time of the substances in the reaction at each reaction interval depending on the change of the concentration of the reactant substance for the chosen chemical process and the given coefficients.

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