MATHEMATICAL MODELING OF A TUBULAR REACTOR. CONTROLLING THE ACTIVITY OF THE CATALYST

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Abstract: The problem of searching the optimal regime and constructive characteristics of the tubular reactor with the ability to control the activity of the catalyst on the length of the tube is considered in this article. The software that allows solving the stated problem has been created on the basis of derived mathematical model.

Notations

C_A, C_B – concentration of raw material and useful product, mole/m^3;

c, c_x – heat capacity of raw products and cooling agent, J/K;

E_i – energy of activation of i-th reaction J/mole;

F – interface of reaction zone and casing, m^2;

G – inlet mass flow of initial mixture, kg/h;

G_x – inlet mass flow of cooling agent, kg/h;

K_i – kinetic constant of i-th reaction, i = 1, 2, 3;

K_{i0} – preexponential factor of i-th reaction;

K_T – heat transfer coefficient, W/(m^2·h);

L – length of reacting zone, m;

l_{chg}, l_{chg1}, l_{chg2} – coordinates of shift in catalyst activity;

Q_i – heating effect of i-th reaction, J/mole;

R – universal gas constant, J/mole·K;

S – specific surface of the catalyst, m^2/m^3;

S_0 – activity of "undiluted" catalyst, m^2/m^3;

$T(l)$ – temperature in reaction zone, K;

$T_x(l)$ – temperature of cooling agent, K;

W_i – speed of i-th reaction, mole/h;

Π – perimeter of tube, m.

Subscripts

c, v, γ – stoichiometric factors.

Often, during the exothermal processes, significant increase in temperatures takes place in the frontal part of catalyst that may adversely affect the output of the end product.

It is possible to remove the overheating of the front part of the reactor by reducing the activity ("diluting") of the catalyst in an overheated zone, i.e. to place an inert into catalyst. It is considered to characterize the rate of "dilution" by function $\varphi(l)$, $0 \leq \varphi(l) \leq 1$. Then catalyst activity distribution by the length of reaction zone will look like

$$S(l) = S_0\varphi(l).$$

The function of diluting will be represented in a polynomial form

$$\varphi(l) = \sum_{i=0}^{n} a_i l^i. \tag{1}$$

We will change catalyst activity distribution by the length of reaction zone by changing an order of a polynomial n and a value of coefficient a_i.

The statement of the problem of determining the optimal concentration fields, temperature fields and catalyst activity will be the following: it is necessary to find such $T(0)$, $C_A(0)$, G, $T_x(0)$, G_x, L, n, a_i, that optimality criterion $I[T(0), C_A(0), G, T_x(0), G_x, L, n, a_i] = C_B(L)$ reaches the maximum at restrictions [1]:

$$\frac{dC_A(l)}{dl} = -\frac{SF}{G}(W_1 + W_3); \qquad \frac{dC_B(l)}{dl} = \frac{SF}{G}(W_1 - W_2);$$

$$\frac{dT(l)}{dl} = \frac{SF}{Gc}\sum_{i=1}^{3}W_iQ_i - \frac{K_T\Pi}{Gc}(T - T_x); \qquad \frac{dT_x(l)}{dl} = \frac{K_T\Pi}{G_xc_x}(T - T_x);$$

$$C_A(0) = C_{A0}; \quad C_B(0) = 0; \quad T(0) = T_0; \quad T_x(0) = T_{x0}; \quad 0 \le l \le L;$$

$$W_1 = K_1\frac{C_B^v}{1 + bC_A^c}; \qquad W_2 = K_2C_A; \qquad W_3 = K_3\frac{C_B^\gamma}{1 + bC_A^c}; \qquad (2)$$

$$K_i = K_{i0}\exp\left(\frac{-E_i}{RT}\right), \quad i = \overline{1, 3};$$

$$S(l) = S_0\varphi(l), \quad \varphi(l) = \sum_{i=0}^{m}a_il^i;$$

$$d_{\min} \le d \le d_{\max}; \quad L_{\min} \le L \le L_{\max};$$

$$C_A(0)_{\min} \le C_A(0) \le C_A(0)_{\max};$$

$$G_{\min} \le G \le G_{\max}; \quad T(0)_{\min} \le T(0) \le T(0)_{\max};$$

$$T_x(0)_{\min} \le T_x(0) \le T_x(0)_{\max}; \quad 0 \le \varphi(l) \le 1.$$

The system (2) has been solved by Runge–Kutta method, search of extremum of optimality criterion has been realized by enumerative technique [2]. The analysis of the received results has shown that temperature difference in the reaction zone had decreased and the output of the end product had increased by 15 % in comparison with $S(l) = S_0$, however it is impossible to load catalyst according to the received solution in real-life conditions. The obtained result should be considered as an upper bound for the theoretically possible yield of the end product.

So, we will represent $\varphi(l)$ in a form of

$$\varphi(l) = \begin{cases} \varphi_1, & \text{if } 0 \le l \le l_{\text{chg}}; \\ 1, & \text{if } l_{\text{chg}} < l \le L. \end{cases} \qquad (3)$$

In this case the reaction zone is presented by two sections with different catalyst activity. The function $\varphi(l)$ will take the form for three sections

$$\varphi(l) = \begin{cases} \varphi_1, & \text{if } 0 \le l \le l_{\text{chg1}}; \\ \varphi_2, & \text{if } l_{\text{chg1}} < l \le l_{\text{chg2}}; \\ 1, & \text{if } l_{\text{chg2}} < l \le L. \end{cases} \qquad (4)$$

Thus, the mathematical model will be analogical to (2), but $\varphi(l)$ will be in a form of (3) for two sections and (4) for three sections.

The yield of the end product has increased by 9 % in comparison with condition $S(l) = S_0$ after realization of diluting function in a form of three sections with different catalyst activity.

This problem has been realized in a software product in the C# programming language. The user can choose the type of the function of diluting, input all source data (Fig. 1) and receive as a result optimal regime and constructive characteristics (Fig. 2) and also diagrams of temperature, concentration and activity of the catalyst distributions on the length of the tube (Fig. 3).

Fig. 1. The window of source data input
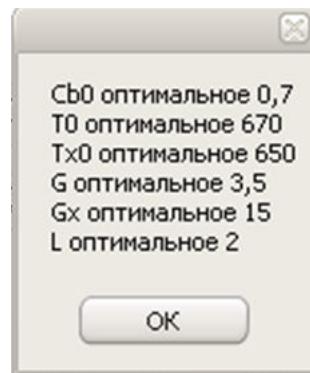
**Fig. 2. The window of optimal characteristics output**
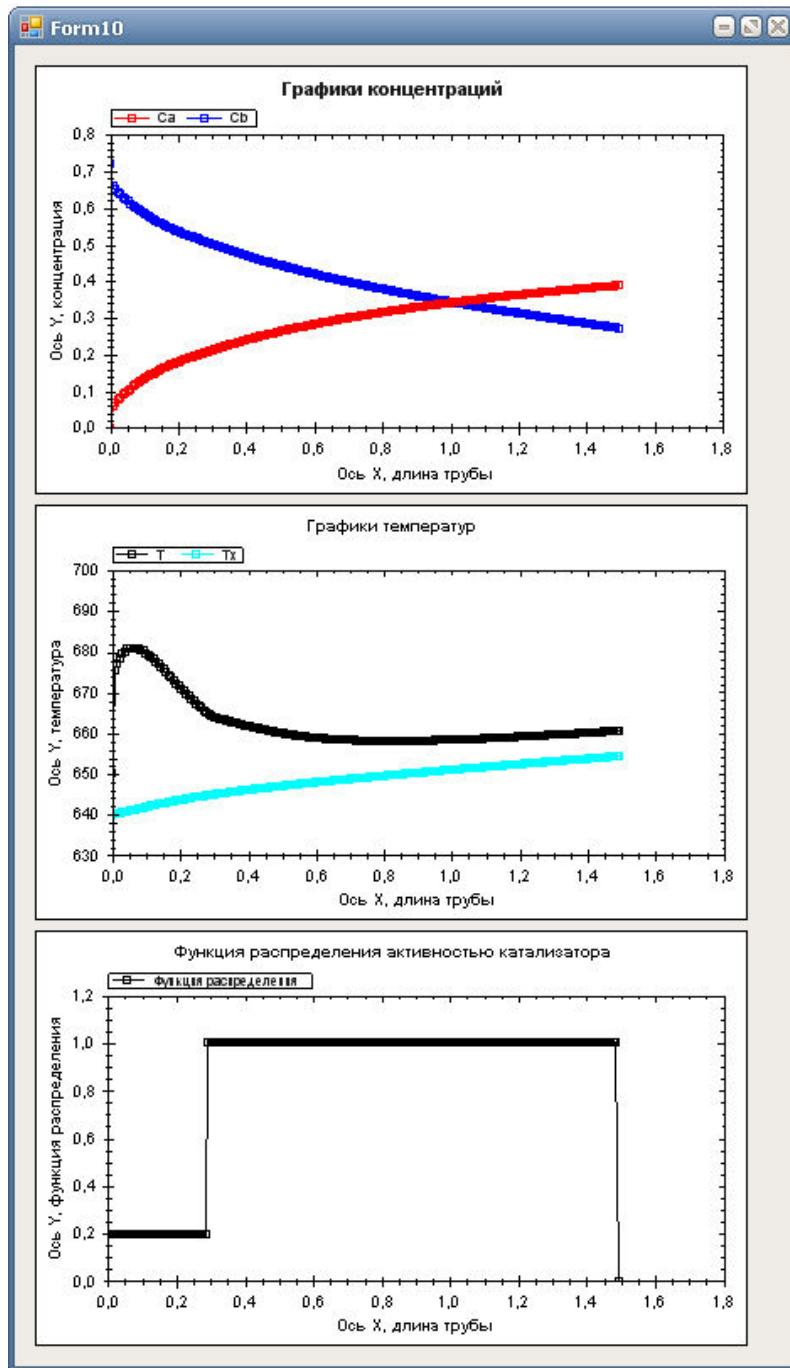
Fig. 3. Diagrams of concentration, temperature and catalyst activity distributions

In conclusion it is necessary to note the varying of catalyst activity distribution by the length of reaction zone allows not only to reduce difference of temperatures, but also to increase the yield of the product.

References

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Математическое моделирование трубчатого реактора. Управление активностью катализатора

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Ключевые слова и фразы: математическое моделирование; трубчатый реактор.

Аннотация: Рассмотрена задача поиска оптимальных режимных и конструктивных характеристик трубчатого реактора с возможностью управления активностью катализатора по длине трубки. Создано программное обеспечение, позволяющее решить поставленную задачу на основе полученной математической модели.

Mathematische Modellierung des Rohrreaktors. Steuerung von der Aktivität des Katalisators

Zusammenfassung: Es ist die Aufgabe des Suchens der optimalen Regimen und konstruktiven Charakteristiken des Rohrreaktors mit der Möglichkeit der Steuerung des Katalisators nach der Länge des Rohres betrachtet. Es ist die Software, die die gestellte Aufgabe auf Grund des erhaltenen mathematischen Modells zu lösen erlaubt, geschaffen.

Modélage mathématique du réacteur tubulaire. Commande de l'activité du catalyseur

Résumé: Est examiné le problème de la recherche des carcatéristiques optimales de régime et de construction du réacteur tubulaire avec la possibilité de la commande de l'activité du catalyseur à travers la longeur du tube. Est créé le logitiel permettant de résoudre le problème posé à la base du modèle mathématique obtenu.

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