The cost’s indicators of the homogeneous reactions in the cascade of perfect mixing reactors prediction by mathematic modelling

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Abstract - One of the typical chemical reactors with a set of nonlinear dynamic characteristics is the perfect mixing reactor of continuous action (PMR-C). In this regard, it is interesting to explore the known process of homogeneous reactions in PMR-C by mathematical means.

Keywords - modeling, cost’s indicators, cascade of perfect mixing reactors, homogeneous reaction.

Introduction

Modeling (in the broadest sense) is one of the basic methods of research in many areas of knowledge as with its help one can provide a reliable assessment of characteristics of quite complex systems. One of the typical chemical reactors is the perfect mixing reactor of continuous action (PMR-C). Of special scientific and practical interest is examining it in real time by the means of mathematical modeling. The development of mathematical model, however, is often gives knowledge about reducing the economic costs of conducting the process. World production of acetic acid is currently over 4.0 million t per year. Acetic acid is one of the basic products of industrial organic synthesis and its derivatives are widely used in food, chemical and other industries. That is why predicting the cost’s indicators of the hydrolysis process of acetic anhydride in PMR-C with the application of modern mathematical models is required.

The Results of the Development

Mathematical model of the dynamics of homogeneous reaction in PMR-C is built based on the thermal and material balance, taking into account volume magnification factor [1] and reaction kinetics [2]. It is represented in the form of equations of a change in the molar share of substance over time and a change in the inner energy of ideal flow of substance.

In this case, the following assumptions are taken into account:
1) physical magnitudes of the substance are constant;
2) total reaction volume is constant;
3) the level of fluid in the reactors is the same;
4) homogeneous reaction is the reaction of first order;
5) flow rate for each of the reactors is the same;
6) thermal consumption for the reactor insulation was neglected.

\[
\frac{dC_{\text{ac,an}(i)}}{d\tau} = \frac{F_i^{\text{in}}C_{\text{ac,an}(i)}(\text{in}) - F_i^{\text{out}}C_{\text{ac,an}(i)}(\text{out})}{\alpha V_{(i)}} - k_0 C_{\text{ac,an}(i)} e^{\frac{-E_A}{RT}},
\]

\[
\frac{dT_{(i)}}{d\tau} = \frac{mc_p(T_0 - T_{(i)}) - \Delta H(T) \cdot k_0 C_{\text{ac,an}(i)} e^{\frac{-E_A}{RT}} + Q_m}{V\rho C_p},
\]

where \( F_i^{\text{in}} \), \( F_i^{\text{out}} \) is the volumetric substance consumption at the inlet and outlet of reactor, respectively, m\(^3\)/h; \( C_{\text{ac,an}(i)}(\text{in}) \) is the concentration of acetic anhydride at the outlet of reactor, mol/m\(^3\); \( C_{\text{ac,an}(i)}(\text{out}) \) is the concentration of acetic anhydride at the inlet to reactor, mol/m\(^3\), \( \alpha = \frac{\sum V_{(i)} / \sum V_{(i)}}{\text{mean weighted value of reaction volume magnification factor, } \cdot} \); \( k \) is the Arrhenius constant, s\(^{-1}\); \( V \) is the reaction volume, m\(^3\); \( \mu_{0,i} \) is the molar inner energy of substance at temperature \( T_0 \), J; \( k \) is the Arrhenius constant, s\(^{-1}\) [3].
Calculation by the model was conducted by the Runge–Kutta method of third order at the following initial data: the number of rectors: one, three, five, ten of total volume 1000 ml, in the temperature range 293 – 410 K.

Table 1
Impact of temperature on the cost of the process of acetic anhydride hydrolysis in the reactor of continuous action

| No. | T, K | Cost, UAH ths. | No. | T, K | Cost, UAH ths. |
|-----|------|---------------|-----|------|---------------|
| 1   | 293  | 9213,68       | 17  | 350  | 2014,93       |
| 2   | 295  | 8056,38       | 18  | 354  | 2087,38       |
| 3   | 297  | 7071,87       | 19  | 358  | 2170,98       |
| 4   | 299  | 6233,96       | 20  | 362  | 2263,40       |
| 5   | 302  | 5204,92       | 21  | 366  | 2362,83       |
| 6   | 306  | 4168,74       | 22  | 370  | 2467,86       |
| 7   | 310  | 3421,32       | 23  | 374  | 2577,38       |
| 8   | 314  | 2886,59       | 24  | 378  | 2690,51       |
| 9   | 318  | 2509,65       | 25  | 382  | 2806,56       |
| 10  | 322  | 2250,58       | 26  | 386  | 2924,99       |
| 11  | 326  | 2080,16       | 27  | 390  | 3045,35       |
| 12  | 330  | 1976,82       | 28  | 394  | 3167,29       |
| 13  | 334  | 1924,57       | 29  | 398  | 3290,53       |
| 14  | 338  | 1911,47       | 30  | 402  | 3414,85       |
| 15  | 342  | 1928,53       | 31  | 406  | 3540,05       |
| 16  | 346  | 1968,96       | 32  | 410  | 3665,98       |

Table 2
Impact of temperature on the cost of the process of acetic anhydride hydrolysis in the cascade of three reactors of continuous action

| No. | T, K | Cost, UAH ths. | No. | T, K | Cost, UAH ths. |
|-----|------|---------------|-----|------|---------------|
| 1   | 293  | 6449,575     | 17  | 350  | 1410,454      |
| 2   | 295  | 5639,467     | 18  | 354  | 1461,166      |
| 3   | 297  | 4950,309     | 19  | 358  | 1519,686      |
| 4   | 299  | 4363,775     | 20  | 362  | 1584,381      |
| 5   | 302  | 3643,444     | 21  | 366  | 1653,983      |
| 6   | 306  | 2918,121     | 22  | 370  | 1727,503      |
| 7   | 310  | 2394,927     | 23  | 374  | 1804,165      |
| 8   | 314  | 2020,616     | 24  | 378  | 1883,356      |
| 9   | 318  | 1756,758     | 25  | 382  | 1964,593      |
Table 3
Impact of temperature on the cost of the process of acetic anhydride hydrolysis in the cascade of five reactors of continuous action

| No. | T, K | Cost, UAH ths. | No. | T, K | Cost, UAH ths. |
|-----|------|----------------|-----|------|----------------|
| 1   | 293  | 5804,618       | 17  | 350  | 1269,409       |
| 2   | 295  | 5075,52        | 18  | 354  | 1315,05        |
| 3   | 297  | 4455,278       | 19  | 358  | 1367,717       |
| 4   | 299  | 3927,397       | 20  | 362  | 1425,943       |
| 5   | 302  | 3279,1         | 21  | 366  | 1488,585       |
| 6   | 306  | 2626,309       | 22  | 370  | 1554,753       |
| 7   | 310  | 2155,435       | 23  | 374  | 1623,748       |
| 8   | 314  | 1818,555       | 24  | 378  | 1695,021       |
| 9   | 318  | 1581,082       | 25  | 382  | 1768,134       |
| 10  | 322  | 1417,868       | 26  | 386  | 1842,742       |
| 11  | 326  | 1310,499       | 27  | 390  | 1918,569       |
| 12  | 330  | 1245,396       | 28  | 394  | 1995,393       |
| 13  | 334  | 1212,481       | 29  | 398  | 2073,036       |
| 14  | 338  | 1204,227       | 30  | 402  | 2151,354       |
| 15  | 342  | 1214,975       | 31  | 406  | 2230,229       |
| 16  | 346  | 1240,448       | 32  | 410  | 2309,568       |

Table 4
Impact of temperature on the cost of the process of acetic anhydride hydrolysis in the cascade of ten reactors of continuous action

| No. | T, K | Cost, UAH ths. | No. | T, K | Cost, UAH ths. |
|-----|------|----------------|-----|------|----------------|
| 1   | 293  | 5456,341       | 17  | 350  | 1193,244       |
| 2   | 295  | 4770,989       | 18  | 354  | 1236,147       |
| 3   | 297  | 4187,962       | 19  | 358  | 1285,654       |
As illustrated in Tables 1-4, the cost of the process of acetic anhydride hydrolysis reduces with changing the temperature from 293 K to 338 K, and then it gradually increases. The optimum is achieved at a temperature 338 K. It is obvious that with the increased volume of the mixture, the reaction rate grows. At the same time, the speed of achieving the necessary degree of conversion decreases. In other words, at the increased reaction volume, the depth of the course of reaction decreases.

**Conclusion**

For the cascade of reactors, the speed of achieving maximum degree of conversion compared with one perfect mixing reactor of the same volume is much higher. In comparison one with three the cost of conducting the process of acetic anhydride hydrolysis decreases considerably, then more moderately, which confirms the recommendation, for considerable reaction volumes in industry, applying the cascade of reactors or the ideal-displacement reactor.

**References**

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