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.

$$\frac{dC_{ac.an.(i)}}{d\tau} = \frac{F_i^{\text{вх}} C_{ac.an.(i)(in)} - F_i^{\text{вих}} C_{ac.an.(i)(out)}}{\cdot \bar{\alpha} V_{(i)}} - k_0 C_{ac.an.(i)} e^{\frac{-E_A}{RT}},$$

$$\frac{dT_{(i)}}{d\tau} = \frac{mc_p (T_0 - T_{(i)}) - \Delta H(T) \cdot k_0 C_{ac.an.(i)} e^{\frac{-EA}{RT}} + Q_{in}}{V \rho C_p},$$

where F_i^{in}, F_i^{out} is the volumetric substance consumption at the inlet and outlet of reactor, respectively, m^3/h; $C_{ac.an.(i)(out)}$ is the concentration of acetic anhydride at the outlet of reactor, mol/m^3; $C_{ac.an.(i)(in)}$ is the concentration of acetic anhydride at the inlet to reactor, mol/m^3, $\bar{\alpha} = \sqrt{\Sigma V_i \alpha_i / \Sigma V_i}$, - mean weighted value of reaction volume magnification factor, -; k is the Arrhenius constant, s^{-1}; V is the reaction volume, m^3; $u_{0,i}$ 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

10	322	1575,409	26	386	2047,492
11	326	1456,11	27	390	2131,744
12	330	1383,773	28	394	2217,104
13	334	1347,201	29	398	2303,373
14	338	1338,03	30	402	2390,393
15	342	1349,972	31	406	2478,032
16	346	1378,275	32	410	2566,187

Table 3

Impact of temperature on the cost of the process of acetic anhydride hydrolysis in the cascade of fife 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

4	299	3691,753	20	362	1340,386
5	302	3082,354	21	366	1399,27
6	306	2468,731	22	370	1461,468
7	310	2026,109	23	374	1526,324
8	314	1709,441	24	378	1593,319
9	318	1486,217	25	382	1662,046
10	322	1332,796	26	386	1732,178
11	326	1231,869	27	390	1803,455
12	330	1170,672	28	394	1875,67
13	334	1139,732	29	398	1948,654
14	338	1131,973	30	402	2022,272
15	342	1142,077	31	406	2096,415
16	346	1166,021	32	410	2170,994

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.

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