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PROCESSES AND DEVICES OF CHEMICAL MANUFACTURES

Temperature Profile in a Displacement Reactor

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Abstract—Results of a mathematical simulation of the heat and mass exchange in the displacement reactor are presented.

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Parameters of a heterogeneous liquid-phase process and the temperature profile in the displacement reactor [1] were defined for 5 types of a non-linear change in a channel temperature *h* with a continuous and discontinuous phase (Fig. 1). We conducted calculations assuming division of 2 mm drops of the dispersed phase in an upper section of the reactor moved from a center to a periphery in the channel narrowing over the height along with the continuous medium while calculations for a bottom section of the reactor (at the continuous flow movement from the periphery to the center in the channel widenning along the height) were performed assuming a fusion of the drops of the dispersed phase.

An increase in a number of the drops of the dispersed phase (of an interfacial area) in the upper section of the reactor partially provided a significant efficiency of transformation (73–78%) of an initial constituent of the dispersed phase for a short residence time in the reactor channel. Also a temperature increase of the medium in the upper reactor section for the first type to 71°C was detected, and for the other 4 types the medium temperature of the uppers section of the reactor was in a range of 54–59°C.

Therefore similarly to [2] using a model of [3] we compute parameters of heterogeneous liquid-phase process with the fast chemical transformation on the more interfacial area due to feeding the dispersed phase of 1 mm drops in the reactor. The dispersed phase and the continuous medium are fed the channel in amount of –0.35, and 1.3 kg/s, respectively. The temperature profile in the reactor channels is computed by an equation of the heat balance for the channel section of a length *dR* with a heat transfer surface *dF* (Fig. 1), and solving the Cauchy limitng-value problem analogously to [2].

We varied non-linearly the height of the channel with the continuous and dispersed phases for 3 types (*1, 2, 3*) of a construction likewise to [2]: $h = aR$, and for 2 types (*4, 4***) linearly $h = a + b\,R$ (see Fig. 1, and the table). Coefficients *a,* and *b* of the channel height *h* denote the hannel narrowing in the upper section, and extension in the bottom section (along the continuous flow).

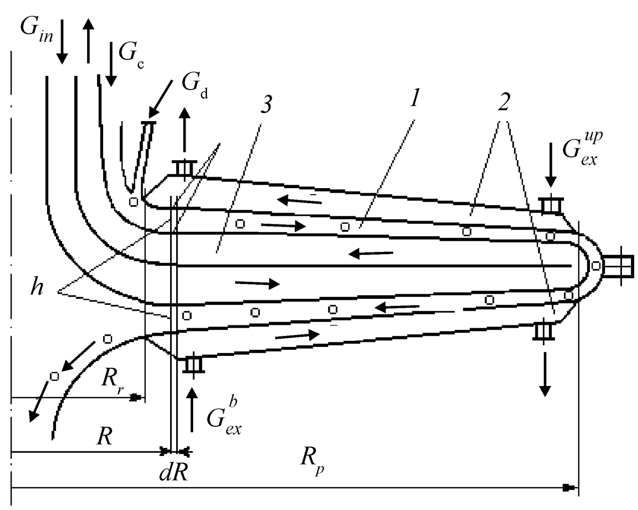

Fig. 1. A scheme of the displacement reactor: (*1*) the channel with dispersed phase G_d and continuous medium G_c ; (*2*) an external upper G_{ex}^{up} and bottom G_{ex}^{b} channels with a cooling agent, (*3*) the internal channel G_{in} with the cooling agent.

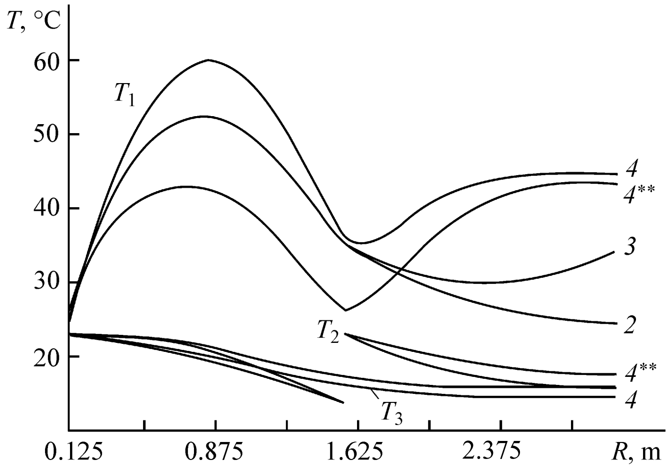

Fig. 2. The temperature change T_1 of the medium, and T_2, T_3 of cooling agent in the reactor channels for *2, 3, 4*, and *4*** types of the construction.

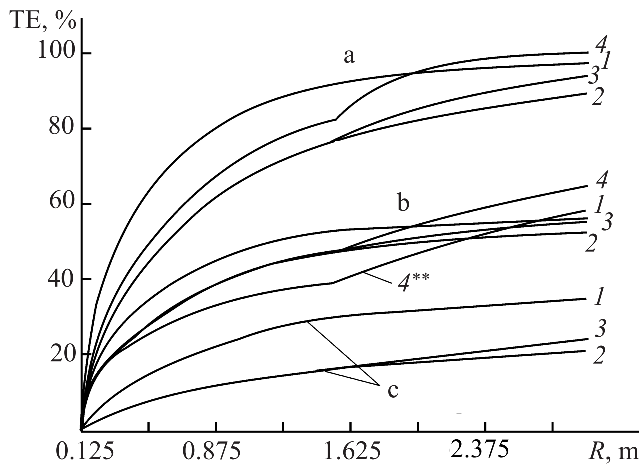

Fig. 3. The change of the transformation efficiency TE of the initial constituents for the dispersed phase and the continuum medium for the *1, 2, 3, 4*, and *4*** types of the reactor construction. (a) In the dispersed phase, (b) in the continuum medium taking into account convective mass transfer (c) without taking into account convective mass transfer.

A solution of the Cauchy problem results in plotting the temperature profile of the medium for the all studied changes of the channel height (Fig. 2, table). The largest value of the environmental temperature 111°C, forbidden according to the technological conditions, was established for the first type of the reactor construction with the continuous flow 0.12–0.13 m/s. An acceleration of the flow (up to 0.77 m/s) due to the narrowing of the start inlet section of the upper channel section in the second type caused decrease in the medium temperature up to 53°C. However, the lesser residence time (16 s) of the medium in the reactor than one in the first type (27 s)

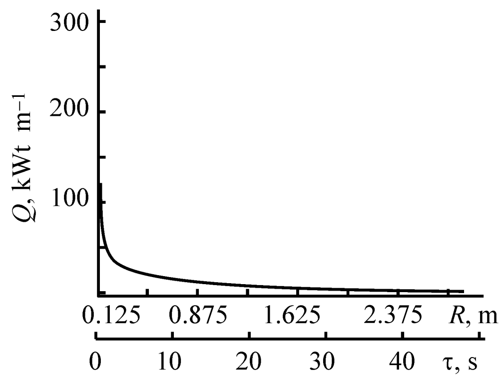

Fig. 4. Change of a density of the heat flow Q in course of the time τ (over a reactor radius R, along the channel with the continuous medium) for the 4th types of the construction.

was insufficient (89%) for the same complete efficiency transformation (97%) of the initial constituent of the dispersed phase (Fig. 1, Table). The increase up to 21 s in the residence time of the retaining the medium in the bottom reactor section in the case of 3rd type results in the some growth (up to 94%) of the transformation efficiency of the initial constituent of the dispersed phase under the same maximum temperature (53°C).

By an increase in the residence time up to 47 s with the help of more gradual narrowing in the upper section of the reactor (and more gradual widening in the bottom section) the transformation efficiency of the initial constituent at the growth of the maximum medium temperature up to 60°C was risen up to 100% in the 4th type with linear change in the channel height.

The calculation of the 1, 2, 3 and 4thes types of the construction did not take into account the convective heat transfer in the continuous media that was sufficiently intense [4] due to high values (about 700 kW, Fig. 4) of the heat flow from the drop surface of the dispersed phase caused by a fast chemical high exothermal reaction (1.3 mJ/kg) of the initial constituents. The calculation of the 4** types taking into account the convective heat transfer shows diminishing maximum temperature of the medium to 43°C with the same practically complete transformation of the initial constituent of the dispersed phase (Fig. 3, table).

At the same time the transformation efficiency of the initial constituent of the continuous medium was not high in comparison with one of the dispersed phase, particularly, at the unaccounted convective mass transfer (Fig. 3, table). Evidently [4] it was caused by lesser molecular and convective diffusion velocity of the constituents for the

Table

Parameters			Type no.				
			non-linear change in the channel height			linear change in the channel height	
			1	*2*	*3*	*4*	*4***
Coefficients of the channel height with the continuous medium: $a \times 10^3$; b		upper section of the reactor	1.63 1	1.13 0.25	1.13 0.25	2.083 0.0007	2.083 0.0007
		bottom section of the reactor	1.63 1	1.13 0.25	1.63 1	14 –0.008	14 –0.008
The height of the channel with the continuous medium *h*, mm: center, periphery		upper section of the reactor	13 1	2 1	2 1	2 1	2 1
		bottom section of the reactor	13 1	2 1	13 1	13 1	13 1
[1]The residence time, s			27	16	21	47	47
*[2]Rate of the process, $SR \times 10^3$, kg/m^{2}s	in the continuous medium	according to initial constituent	533	854	854	837	737
		according to product	457	769	769	937	592
	in the dispersed phase	according to initial constituent	193	193	193	193	193
		according to product	219	219	219	219	219
*[3]The transformation efficiency *TE, %*	continuous medium		56	53	56	65	58
	dispersed phase		97	89	94	100	100
*[4]Temperature of the medium, °C			111	53	53	60	43
*[5]Temperature of the output medium , °C			24	25	34	45	43
*[6]Temperature of the cooling agent at the channel inlet, °C		upper external inlet	12	15	15	15	14
		bottom external inlet	16	14	13	16	16
		internal inlet	13	15	15	16	15
*[7]The cooling agent flow at the channel inlet, kg/s		upper external inlet	3.8	3.5	3.5	3.6	3.5
		bottom external inlet	1.0	1.3	1.2	1.2	1.0
		internal inlet	5.5	5.5	5.5	5.5	5.5

[1–7] The values were measured at the temperature of 25°C of the continuous medium at the channel inlet, and of 23°C of the cooling agent at the channel outlet.
* The maximum values.
** The values taking into account the conversion heat transfer.

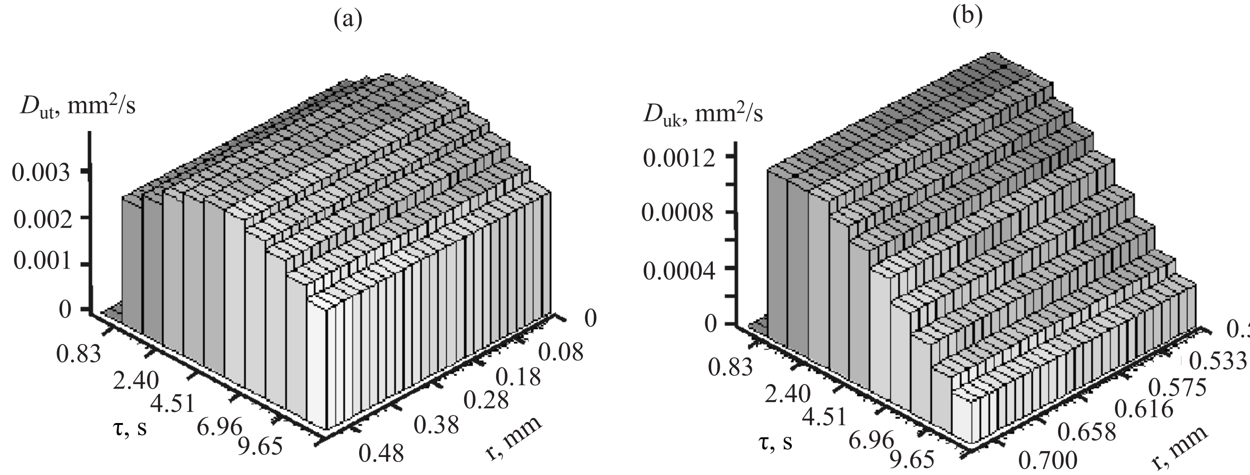

Fig. 5. Change in the distribution of the molecular $D_{ic.m}$ and convective $D_{ic.v}$ diffusion coefficients (a) of the dispersed phase, and (b) of the continuous medium over the radius r of the dispersed phase drop, and of a layer of the continuous medium wrapping the drop in the course of the time τ for the upper section of the 4th type of the reactor construction.

continuous medium than for the dispersed phase (Fig. 5) as the viscosity of the continuous medium was larger. A size and a molecular structure of the diffusing constituents also effect on the diffusion velocity.

Coefficients of the convective diffusion of the initial constituent D_{ic} and of the reaction product D_p in the continuous medium, and also in the dispersed phase were computed as k-fold increase in the coefficients of their molecular interdiffusion ($D_{uk}=kD_u$, $D_{ek}=kD_e$) calculated according to the following equation [4]:

$$D_u = 7.4\times 10^{-8}\left(\frac{T}{\mu_e Vm_u^{0.6}}\right)\left(p_{as}Mm_e\right)^{0.5},$$

$$D_e = 7.4\times 10^{-8}\left(\frac{T}{\mu_u Vm_e^{0.6}}\right)\left(p_{as}Mm_u\right)^{0.5},$$

where: V_m was the molecular volume, cm^3/mol, M_m, molecular weight, g/mol, μ, the dynamic viscosity coefficient of the diffusing component, MPa, T, the temperature, °C; p_{as}, was an association parameter, l; indices of u and p denote initial component and reaction product, respectively.

A coefficient of the enlargement k was calculated in the dependence on a relative increment of the heat flow density according to equation:

$$k = k^{\max} - (k^{\max} - 1)\left(\frac{Q^{\max} - Q(\tau)}{Q^{\max}}\right)^{p},$$

where $Q($ $)$, $Q^{\max}$ are the current and maximum values of the heat flow density, Wt, k, $k^{\max}$ are current and maximum (at $Q( ) = Q^{\max}$) values of the coefficient of enlargement, p is an exponent taking into account a rate of diminishing the heat flow density (an effect of the heat generation on the convective diffusion velocity in the continuous medium). The computation was performed at $k^{\max}=30$, $p_u=1.9$, $p_e=1.0$.

More accurate simulation of the effect of the heat generation on the process enhancement in the continuous medium necessitates more detail modeling the heat and mass exchange that is a subject of the forward studies. However on the basis of the obtained results we can provide the acceptable temperature of the medium at reasonable maximum in the linear narrowing (widening) along the channel height according to the technological conditions using water as the cooling agent fed gently in the reactor channels.

REFERENCES

1. USSR Patent 324322, 1991.
2. Zheranin, A.V., *Khim. Prom.*, 2007, no. 3, pp. 151–155.
3. Zheranin, A.V. and Ovcharenko, A.G., *Izvestiya Vuzov, Ser. Khimiya & Khimicheskaya Tekhnologiya*, 2005, vol. 12, no. 48, pp. 89–91.
4. Sherwood, T. et al., *Mass Transfer*, McGraw-Hill Inc., 1975.