UDC 669.046:536.24.001.57

V.A. Skachkov [(1)], associate professor, c.t.s.
V.I. Ivanov [(1)], senior research worker
A.G. Kirichenko [(1)], associate professor, c.t.s.
A.V. Skachkov [(2)], deputy director

MODELLING OF MASS TRANSFER PROCESS FOR REACTIONARY GASES AND PYROCARBON AT COMPACTION OF CARBON COMPOSITES IN REACTORS OF RUNNING TYPE

[(1)] Zaporozhe state engineering academy, Ukraine,
[(2)] OAJ «Giros», Zaporozhe, Ukraine

It is executed mathematical modeling of mass transfer for mixture of reactionary gases and deposition of pyrolytical carbon in the thermochemical reactors of running type at the isothermal compression of porous carbon composites. A model takes into account the processes of transporting of gaseous hydrocarbons in the porous structure of composite, their subsequent decomposition and deposition of pyrolitical carbon on the heated surfaces of pores.

Keywords: carbon composite, reactionary gas, mass transfer, pyrolytical carbon, isothermal compression, running reactor, modeling

At the production of carbon compos major redistribution there is a compression of porous structure carbonplastic with the use of natural gas (methane) [1]. At passing of homogeneous processes the complex of hydrocarbons, and also row of radicals [2-4]. Foods of homogeneous reactions and initial hydrocarbon diffuse to the heated surfaces carbonplastic and in his porous structure with subsequent decomposition on the heated walls of pores and formation of hard phase – pyrocarbon.

In the conditions of motion of gas streams along the axis of reactor and trifle of speed of diffusion as compared to speed of streams equalization of transfer of mass i component of mixture of reactionary gases in the conditions of chemical transformation appears in a kind:

$$\frac{\partial C_i}{\partial \tau} = \operatorname{div}\left(\overline{V} \cdot C_i - D_{iN} \cdot \Delta C_i\right) = k_i \cdot C_1^n \cdot C_2^n ... C_N^n \ , \qquad (1)$$

where $C_i = C_i\left(\overline{x}, \tau\right)$ is a concentration of i component of mixture of reactionary gases; $\vec{x}$ is radius-vector of the examined point of volume of reactor; D_{iN} is a coefficient of diffusion of i component from mixture of N components; ΔC_i is a gradient of concentration; k_i is a constant of speed of homogeneous reaction on i component; n is an order of reaction on i component.

Between's by the concentrations of i component of reactionary mixture in the volume of reactor (C_i^0) and on the surface of porous material (C_i^S) looks like

$$C_i^0 = \frac{\beta \cdot C_i^0}{\left[\beta + \left(1 - \omega_i\right) \cdot k_i^S - \pi \cdot \omega_i \cdot \left(\frac{2k_i^S \cdot r}{D_i}\right)\right]} \ , \qquad (2)$$

where β is a constant of speed of diffusion, $\beta = D_i / \delta$.

For simplification of decision of the system of equalizations (2) entered the

row of assumptions [5]:

– examined a circular axisymmetrical reactor, for which a function, describing the structure of gas streams, does not depend on a circuitous co-ordinate, and office hours are stationary;

– speeds of homogeneous and heterogeneous reactions on every individual component correspond to the first order;

– at the decision of task applied the method of равнодоступных surfaces of Frank-Khamenetsky.

Then the system of equalizations (1) can be written down in a kind

$$\frac{d\left(UC_i\right)}{dz}+\frac{2k_i^S\cdot C_i^S}{R\cdot\left[\beta+\left(1-\omega_i\right)\cdot k_i^S-\pi\cdot\omega_i\cdot\left(\frac{2k_i^S\cdot r}{D_i}\right)\right]}=W_i^S\ , \tag{3}$$

where U is speed of gas stream on the axis of reactor; R is a radius of reactor; z is a co-ordinate axis, directed on the axis of reactor.

The concentrations of foods of homogeneous-heterogeneous reactions in a running reactor determine with the use of correlations, resulted in work [5], constants of speeds of chemical reactions of formation of foods of these reactions - on correlations of work [6]:

Task about mass transfer in a single cylindrical pore carbonplastic it is possible to formulate as follows:

$$\frac{d^2C_i}{d\ell^2}=\frac{2k_i^s\cdot C_i}{\overline{r}\cdot D_i}\ ; \tag{4}$$

$$\vartheta\cdot\frac{d\rho}{d\ell}=\sum_{i=1}^{N}S_i\cdot k_i^s\cdot C_i\ ; \tag{5}$$

$$C_i\big|_{\ell=0}=C_i^0\ ; \tag{6}$$

$$\left.\frac{dC_i}{d\ell}\right|_{\ell=h}=0\ ; \tag{7}$$

$$\rho\big|_{\ell=0}=\rho_0\ , \tag{8}$$

where $\overline{r}$, ℓ are a depth and middle radius and depth of pore accordingly; $2h$ is a thickness of good; S_i is a specific reactionary surface of compo; ρ_0 is an initial closeness of material of composite; ϑ is speed of height of pyrolytical carbon; N is an quantity of reactive components in the volume of reactor.

Decision of equation (4) taking into account terms (6)-(7) it is possible to present as expressions:

$$C_i=\frac{C_i^0\cdot\left\{\exp\left[\left(\frac{2k_i^s}{\overline{r}\cdot D_i}\right)^{0,5}\cdot\left(\ell-2h\right)\right]+\exp\left[-\ell\cdot\left(\frac{2k_i^s}{\overline{r}\cdot D_i}\right)^{0,5}\right]\right\}}{1+\exp\left[2\cdot\ell\cdot\left(\frac{2k_i^s}{\overline{r}\cdot D_i}\right)\right]}, \tag{9}$$

In connection with that size of specific reactionary surface carbonplastic S_i corresponds to the specific surface of pores, she can be defined on correlation:

$$S_i = \frac{2(\rho_r - \rho)}{\overline{r} \cdot \rho_r \cdot \rho}, \qquad (10)$$

where ρ_r is a real closeness of material carbonplastic.

After the substitution of expression (10) in differential equation (5) will have:

$$\frac{d\rho}{d\ell} = \frac{2(\rho_i - \rho)}{\overline{r} \cdot \rho_i \cdot \rho} \cdot \sum_{i=1}^{N} h_i \cdot C_i \cdot \frac{\rho_0}{\sum_{i=1}^{N} k_i^s} \qquad (11)$$

Subsequent integration of expression (11) on ρ (from ρ_0 to ρ and on ℓ (from 0 to ℓ) allows to get transcendent equation in relation to a parameter ρ, characterizing the change of seeming closeness of material carbonplastic on the thickness of his wall: For realization of calculable experiment with the use of the offered mathematical model the computer program is worked out in language of TURBO-PASKAL.

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