Eqs. (5) and (6), temperature-dependent; τ, corrected temperature; b_i, h_i, coefficients of polynomials in (7); c_p, specific heat at constant temperature; c_{p_1}, v_1, parameters of a point at a given isotherm for a selected pressure p_1; B', H' and B", H", first and second temperature derivatives of coefficients B and H according to (7).

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CALCULATING THE TIME OF ISOTHERMAL SATURATION OF A SPHERE

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UDC 533.73:536.42

Results of a numerical solution of the inverse Stefan problem are presented for a sphere with boundary conditions of the third kind. Expressions are derived for calculating the time of total diffusion saturation of a spherical core, taking into account the rate of interaction of the gas phase with the surface of the solid.

In many fields of technology it is important to know the time of isothermal diffusion saturation of solid particles whose material is used to form a target product. A characteristic case is provided by saturation of particles of spherical form and separation of the original material from the target product by a moving boundary of phase separation. Usually, the diffusing matter penetrates the solid from a gaseous or liquid phase. The depth of saturation is determined by the rate of mass transfer in the solid and in the surrounding medium. The diffusion coefficient in the liquid or gas is many orders greater than in the solid. Therefore, in the first approximation of the process description we can confine ourselves to the solution of the interior problem of mass transfer, i.e., to the analysis of the reaction diffusion within the solid.

The problem concerned with diffusion saturation of a sphere for an arbitrary kinetic relationship of the motion of the phase separation boundary is solved in [1, 2]. However, the use of the methods of these investigations, to determine the depth of saturation of the sphere, i.e., the solution of the inverse problem, constitutes considerable difficulties. We have made an attempt to numerically solve the problem of isothermal saturation of a sphere-shaped particle as a result of a reaction diffusion within the solid phase, taking into ac-

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TABLE 1. Results of Calculating the Saturation Time for Given Positions of the Boundary $y(t)R^{-1}$ and the Parameters μ and ε

$y(t)R^{-1}$	$\mu=10;\ \varepsilon=1,0$	$\mu=10^2;\ \varepsilon=1,0$	$\mu=10^3;\ \varepsilon=1,0$	$\mu=1,0;\ \varepsilon=1,0$	$\mu=10^{-2};\ \varepsilon=1,0$	$\mu=10^{-1};\ \varepsilon=1,0$	$\mu=10^{-3};\ \varepsilon=1,0$	$\varepsilon=10^{-2};\ \mu=10^3$	$\varepsilon=10^{-2};\ \mu=10^2$	$\varepsilon=10^{-2};\ \mu=10$	$\varepsilon=10^{-2};\ \mu=1$	$\varepsilon=10^{-2};\ \mu=10^{-1}$
	τ						τ					
1,0	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,9	0,025	7,015	69,875	0,100226	0,01671623	0,025057	0,01579513	82,1398	8,2285	0,835788	0,105558	0,022504
0,8	1,521	14,708	146,55	0,1989501	0,03455934	0,051692	0,0327159	156,2577	15,64588	1,588872	0,1830936	0,0424469
0,7	2,168	20,772	206,76	0,2946697	0,0612207	0,0858260	0,0586062	214,1829	21,45061	2,186296	0,2598355	0,0696466
0,6	2,688	25,406	252,49	0,3860641	0,0945635	0,1254570	0,0913168	257,7259	25,83887	2,646099	0,3266731	0,097202
0,5	3,101	28,881	285,74	0,4718101	0,132389	0,1684039	0,1286343	289,1341	29,0093	2,986352	0,3836047	0,125590
0,4	3,425	31,217	308,52	0,5504736	0,1723998	0,2124745	0,1682438	310,5988	31,16075	3,225189	0,4306278	0,1530101
0,3	3,675	32,814	322,87	0,6203716	0,2121173	0,2553058	0,2076578	323,6633	32,49026	3,380839	0,4677366	0,1776604
0,2	3,861	33,810	330,85	0,6793321	0,2487417	0,2941939	0,2440627	330,5424	33,19848	3,471689	0,494918	0,1977383
0,1	3,989	34,381	334,56	0,7241278	0,27837	0,3282251	0,2739153	333,2104	33,48632	3,516100	0,5121359	0,2114347
0,0	$40,57=\tau^*$	$34,638=\tau^*$	$335,92=\tau^*$	$0,7482460=\tau^*$	$0,2960992=\tau^*$	$\tau^*=0,3436985$	$\tau^*=0,2912056$	$\tau^*=333,7021$	$\tau^*=33,5534$	$\tau^*=3,530497$	$\tau^*=0,519210$	$0,216882=\tau^*$

$y(t)R^{-1}$	$\mu=10^3;$ $\varepsilon=10^{-1}$	$\mu=10^2;$ $\varepsilon=10^{-1}$	$\mu=10;$ $\varepsilon=10^{-1}$	$\mu=1;$ $\varepsilon=10^{-1}$	$\mu=10^3;$ $\varepsilon=10^{-0,5}$	$\mu=10^2;$ $\varepsilon=10^{-0,5}$	$\mu=10;$ $\varepsilon=10^{-0,5}$	$\mu=10^{-3};$ $\varepsilon=10^{0,5}$	$\mu=1;$ $\varepsilon=10^{0,5}$	$\mu=10^{-1};$ $\varepsilon=10^{0,5}$	$\mu=10^{-3};$ $\varepsilon=10^2$	$\mu=10^{-4};$ $\varepsilon=10^2$
	τ						τ					
1,0	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,9	82,14257	8,230062	0,936200	0,0968064	82,08744	8,23225	0,837204	0,0156705	0,107584	0,095138	0,024311	0,02411
0,8	162,8218	15,6485	1,590714	0,184675	156,2380	15,65399	1,591112	0,0304311	0,227187	0,045341	0,067278	0,066839
0,7	219,3241	21,45714	2,190864	0,263477	214,0534	21,46871	3,220172	0,052229	0,353035	0,0846897	0,1354689	0,134810
0,6	261,806	25,85126	2,655114	0,333164	257,7154	25,87432	2,67610	0,0790243	0,481189	0,134869	0,225186	0,224332
0,5	292,1645	29,02962	3,002024	0,3936641	289,1850	29,07085	3,037549	0,108791	0,608245	0,193256	0,3323191	0,3312928
0,4	312,5241	31,19221	3,25046	0,4448677	310,4477	31,26177	3,30513	0,139474	0,730825	0,256797	0,4521330	0,4509580
0,3	324,9387	32,54169	3,419266	0,4865996	323,5347	32,65448	3,49671	0,168965	0,845184	0,322042	0,5788944	0,5775939
0,2	331,3296	33,28319	3,526453	0,5185586	330,5263	33,45665	3,62748	0,195038	0,946642	0,384759	0,70507	0,7036680
0,1	333,7939	33,60022	3,587264	0,5401711	333,4293	33,86022	3,70832	0,2151794	1,028300	0,439013	0,819176	0,8176997
0,0	$\tau^*=334,2940$	$\tau^*=33,72636$	$3,611281=\tau^*$	$\tau^*=0,5502538$	$\tau^*=334,2104$	$\tau^*=34,00308$	$\tau^*=3,74324$	$\tau^*=0,225804$	$\tau^*=1,075584$	$\tau^*=0,473111$	$\tau^*=0,895810$	$\tau^*=0,894295$

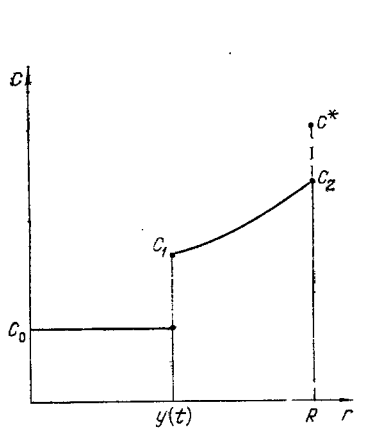

Fig. 1

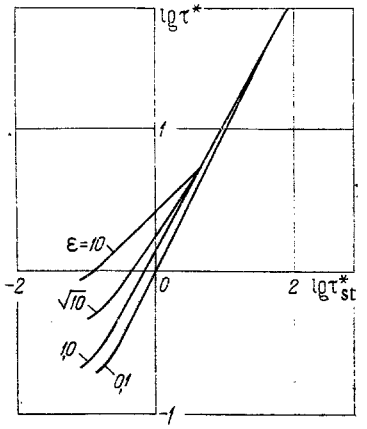

Fig. 2

Fig. 1. Scheme of concentration distribution in the case of reaction diffusion in a sphere.

Fig. 2. Dependence of $\tau^*(\varepsilon, \mu)$ on $\tau^*_{st}(\mu)$.

count the surface chemical reaction, and to approximately describe this solution in a form that is convenient for practical use.

In Fig. 1 we have shown a given distribution of the concentration of the diffusing matter. In accordance with the course of saturation we assume that first the particle is saturated uniformly over the entire volume up to a certain limiting concentration C_1 which is determined by the diffusing material. After this, a layer of the target product is simultaneously and uniformly formed on its surface and grows toward the center. The depth of saturation of the sphere is determined by the sum of the times of these stages of the process. The duration of the uniform saturation of the sphere up to the concentration C_1 can be determined by the methods [3, 5]. Therefore, the time count of saturation is taken from the instant when the growth of the layer of the target product starts.

The problem being considered is a nonlinear problem of mathematical physics with a moving phase separation boundary, and determination of the position of this boundary is necessary for its solution.

The problem is formulated by the equation

$$C_t = D(C_{rr} + 2r^{-1}C_r) \tag{1}$$

with the conditions

$$\begin{gathered} K[C^* - C(R, t)] = DC_r(R, t);\ C[y(t), t] = C_2; \\ -DC_r(y, t) = (C_2 - C_1)\dot{y}(t);\ y(0) = R, \end{gathered} \tag{2}$$

where the first expression in (2) describes the emergence of the diffusing matter from the surrounding medium in the form of the boundary condition of the third kind, and the second describes the condition on the moving boundary. Here K — the constant of heterogeneous chemical reaction — is regarded as independent of the concentration, which is valid in a fairly broad interval of variation of the parameters [7].

We introduce the dimensionless variables

$$\begin{gathered} X = 1 - rR^{-1};\ \tau = (C^* - C_2)(C_2 - C_1)^{-1} DtR^{-2};\ Z = 1 - y(t)R^{-1}; \\ U = [C^* - C(r, t)](C_2 - C_1)^{-1};\ \varepsilon = (C^* - C_2)(C_2 - C_1)^{-1};\ \mu = D(KR)^{-1}. \end{gathered} \tag{3}$$

Then (1) and (2) are transformed into

$$U_{XX} - 2(1 - X)^{-1}U_X = \varepsilon U_\tau, \tag{4}$$

$$U(0, \tau) = \mu U_X(0, \tau);\ U(Z(\tau), \tau) = 1;\ U_X(Z(\tau), \tau) = Z_\tau;\ Z(0) = 0. \tag{5}$$

It is expedient to consider the quasistationary case of the problem (4), (5). Here $\varepsilon = 0$ and Eq. (4) is integrated with the condition (5) in the form

$$\tau_{\varepsilon=0} = 0.5(1 - Z^2) + 3^{-1}(\mu - 1)(1 - Z^3). \tag{6}$$

The time of total diffusion saturation of a sphere is given by the expressions

$$\tau^*_{\varepsilon=0} = 6^{-1}(2\mu + 1), \tag{7}$$

$$t^*_{\varepsilon=0} = \left(\frac{C_2 - C_1}{C^* - C_2}\right)\frac{R^2}{6D}(2DK^{-1}R^{-1} + 1). \tag{8}$$

From (8) it follows that inside the diffusion region, where the rate of the process is checked, the time of total saturation is proportional to R^2, while in the kinetic region of reaction it is proportional to R.

In the general form the problem (4), (5) was solved numerically on a Minsk-32 computer. The method of finite elements in a grid in the plane with the variables X and τ was used. Along the X axis a constant step of 10^{-4} was specified with respect to the variable τ. A noniterative scheme was used to solve the resulting difference equations. The accuracy check of the numerical solutions and the choice of the step length were effected by comparing the results of the calculation with the exact solution for the limiting values of the parameters μ and ε.

The results of the calculation of values of τ for given positions of the moving boundary $y(t)R^{-1} \in [1, 0]$ with a step of 0.1 are presented in Table 1.

In Fig. 2 we have shown the calculated dependence of the time $\tau = \tau(0, \varepsilon, \mu)$ of total isothermal saturation of a spherical particle, being the fundamental characteristic for obtaining a pure target product, on the value $\tau^*_{\varepsilon=0}$, given by (7). The lines from the family $\tau^*(\tau^*_{\varepsilon=0})$ have a small curvature and a broad range of variation of the values μ and ε. This signifies that the function $\tau^*(\varepsilon, \mu)$ weakly depends on the magnitude of the parameter ε. Therefore, the approximation of numerical values τ^* can be sought in the form

$$\tau^* \cong \tau^*_{\varepsilon=0}\sum_{m=0}^{\infty} A_m \varepsilon^{m/2}. \tag{9}$$

The first approximation for (9), which ensures an error not greater than 20% for the entire set of calculation results $10^{-3} \leqslant \mu \leqslant 10^4$, $0 \leqslant \varepsilon \leqslant 10^2$, equals

$$\tau^* \cong 6^{-1}(2\mu + 1)[1 + 0.5\varepsilon^{1/2}(2\mu + 1)^{-1/2}]. \tag{10}$$

From this feature of the function $\tau^*(0, \varepsilon, \mu)$ it follows that the function $Z(\tau)$ can be sought as the solution of the equation obtained by means of [8]:

$$1 - (1 + \mu)\sum_{n=0}^{\infty}[(2n + 2)!]^{-1}\frac{\partial^n}{\partial\tau^n}[(1 - Z)Z_\tau^{2n+2}] = \sum_{n=0}^{\infty}\varepsilon^n[(2n + 2)!]^{-1}\frac{\partial^n}{\partial\tau^n}[(1 - Z)Z_\tau^{2n+2}] \tag{11}$$

in the form of the series $Z(\tau) = \sum_{m=0} Z_m \varepsilon^m$ for $\varepsilon > 0$.

NOTATION

$C(r, t)$, concentration of diffusing matter in the layer of target product; C_1, C_2, solubility of diffusing matter in the material of a spherical particle and its minimum solubility in the target product, respectively (see Fig. 1); C^*, concentration of diffusing matter in the adsorptive layer determining its emergence from the medium surrounding the particles; D, coefficient of reaction diffusion; t, time of reaction diffusion (of isothermal saturation of the sphere); r, position vector with its origin at the center of the sphere; $y(t)$, modulus of the position vector characterizing the position of the boundary between the target product at the time t; $\dot{y}(t)$, velocity of the moving boundary; τ^*, t^*, dimensionless and dimensional time of total diffusion saturation, respectively.

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METHODS AND PROSPECTS OF THE DIRECT EXPERIMENTAL VERIFICATION AND REFINEMENT OF THE "PACKET" MODEL OF EXTERNAL HEAT TRANSFER IN A FLUIDIZED BED

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Analysis of the Basis of the Model

The packet model proposed by Mickley [1] has served as a basis for explaining a whole series of special characteristics of external heat transfer in fluidized beds and for the construction of engineering formulas facilitating the practical estimation and calculation of heat-transfer coefficients. After considering new experimental data as to the structure of the boundary zone [2, 3] and the sharp criticism of the packet model made by Syromyatnikov [4], a more detailed analysis of the fundamental principles of the model has now become a matter of great importance.

A fluidized bed of solid particles agitated by a rising gas flow is usually very inhomogeneous, not only in the boundary zone, but also over the whole volume of the apparatus. The local porosity ε fluctuates constantly from $\varepsilon = 1$ to $\varepsilon = \varepsilon_{min} \approx 0.4$. In order to describe a number of phenomena associated with heat and mass transfer and catalytic reactions, many research workers [5] prefer to consider these fluctuations schematically and (by way of simplification) to assume that at any specific instant the fluidized bed consists of regions existing in one of two limiting states: $\varepsilon = 1$, i.e., gas bubbles free from particles, and $\varepsilon = \varepsilon_{min}$, constituting the so-called dense or compact phase (packets). The basis for making such a far-reaching schematization when analyzing catalytic reactions in a fluidized bed is the vast quantitative (practically qualitative) difference in the properties of these limiting states. Inside the bubble the gas never encounters catalyst grains, and no reaction occurs. In the dense phase, however, the reaction rate reaches a maximum. To a first approximation this so-called two-phase model of the fluidized bed gives a satisfactory explanation for the reduction in the yield of the reaction in a fluidized bed by comparison with a stationary catalyst and also reveals the main factors capable of influencing the degree of yield. Later on, however, when attempting to refine the quantitative laws of the process [6], it was found necessary (to a certain extent) to allow for intermediate states as well, namely, particles spilling down into the interior of the bubble, the "tail" of the bubble, and the "cloud" of adjacent particles undergoing vigorous gas-exchange with the bubble itself. It may well be that a description of the processes based on a fuller account of all the continuously varying states existing between the bubble and the packet will lead to major advances [7].

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