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HEAT AND MASS TRANSFER IN COMMERCIAL DESORBERS WITH A HEATING SURFACE
IN THE FORM OF A VERTICAL TUBE BUNDLE
AND A THERMOFLUIDIZED HEAT-CARRIER BED

A. P. Nesenchuk, A. M. Gabriél', E. N. Antonishina,
V. A. Sednin, A. A. Sklyar, and L. V. Shaton

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A mathematical model is presented of heat and mass transfer in a thermofluidized bed in the thermal regeneration of synthetic zeolites. Theoretical data are compared with experimental results.

This article is a continuation of the work done in [1, 4] on the use of thermofluidization to intensify heat and mass transfer in the regeneration of synthetic zeolites of CaA, MgA, and other aluminates in processing equipment at machine-building plants.

The regime of thermofluidization of a flow of disperse sorbent during its heating begins when evolution of the gaseous sorbate becomes so intense that the velocity of the gas phase exceeds the initial fluidization velocity. The properties of the disperse flow change abruptly at this moment, mixing becomes intense, and there is a significant increase in the effective thermal conductivity of the bed in the thermofluidization zone. It is difficult to calculate the thermofluidization regime due to the nonlinearity of the corresponding model.

Here we use a model of a descending flow moving past a vertical cylindrical heater. We use the approximation that the medium is continuous and has effective properties which model dense and thermofluidized flow. The numerical solutions obtained can then be used to obtain an engineering optimization of commercial units to extract carbon dioxide and other gaseous sorbates from a gas suspension.

We will examine an annular vertical channel (Fig. 1) R_0 with a cylindrical internal heater of radius r_0 . The rectangular region BCDE and its longitudinal section are the two-dimensional calculation region, with the coordinate origin at point A. A zeolite flow G crosses section BC with a specified degree of adsorption α_0 and an initial temperature T_0 . The boundary CD is thermally insulated and nonpermeable to the gas and solid phase. The boundary BE is heated by the heat flow Q and is also nonpermeable. The porosity ε_0 on the boundary DE is equal to the porosity of the dense flow ($\varepsilon_0 = 0.4$), since there is a gas seal here and gas evolution is directed upward toward section BC. The gas flow increases during ascent and, beginning at a certain section, the bed of sorbent is fluidized.

The sought functions are: the temperature of the flow $T(r, X)$, the porosity of the flow $\varepsilon(r, X)$, and the degree of adsorption $\alpha(r, X)$.

In the approximation of a continuum with uniform adsorption and a negligibly short thermal relaxation time, the flow is described by the system of equations (in the region $r_0 \leq r \leq R_0$; $0 \leq X \leq X_0$):

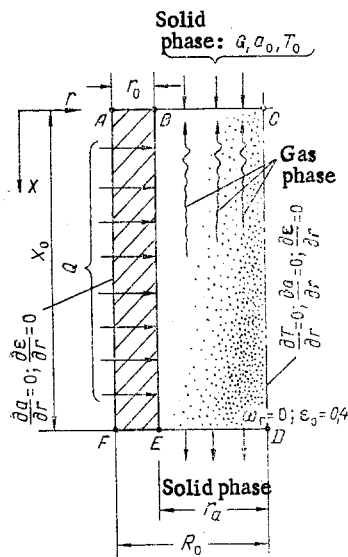


Fig. 1

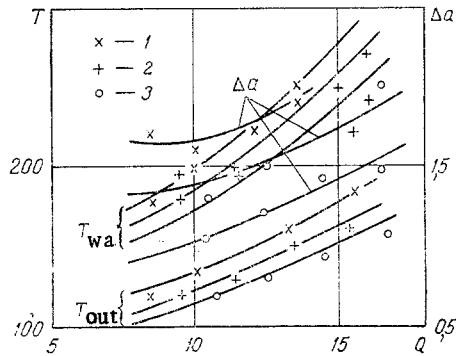


Fig. 2

Fig. 1. Geometry of desorber with thermofluidized bed.

Fig. 2. Relationship between temperatures of tube wall T_{wa} and zeolite at the bundle outlet T_{out} , reduction in degree of adsorption $\Delta\alpha$, and heat release from the surface of the tube bundle: 1) zeolite flow rate in desorber 1.8; 2) 2.2; 3) 2.5 $\text{kg}/\text{m}^2 \cdot \text{sec}$. T , $^{\circ}\text{C}$; Q , kW/m^2 ; $\Delta\alpha$, %.

$$\rho_g \frac{\partial (w_g \epsilon)}{\partial X} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho_g D_e \frac{\partial \epsilon}{\partial r} \right) + I [a - a(T)] \rho_d (1 - \epsilon); \quad (1)^*$$

$$G \frac{\partial a}{\partial X} = \frac{1}{r} \frac{\partial}{\partial r} [r \rho_g (1 - \epsilon)] D_a \frac{\partial a}{\partial r} - I [a - a(T)] \rho_d (1 - \epsilon); \quad (2)$$

$$(c_d + ac_g) G \frac{\partial T}{\partial X} = \frac{1}{r} \frac{\partial}{\partial r} [r \rho_g (1 - \epsilon)] (c_d + ac_g) D_T \frac{\partial T}{\partial r} - IH [a - a(T)] \rho_d (1 - \epsilon) \quad (3)$$

with the initial conditions

$$T|_{X=0} = T_0; a|_{X=0} = a_0; \epsilon|_{X=X_0} = \epsilon_0 \quad (4)$$

and boundary conditions

$$\left. \frac{\partial T}{\partial r} \right|_{r=R_0} = \left. \frac{\partial \epsilon}{\partial r} \right|_{r=R_0} = \left. \frac{\partial a}{\partial r} \right|_{r=R_0} = \left. \frac{\partial \epsilon}{\partial r} \right|_{r=r_0} = \left. \frac{\partial a}{\partial r} \right|_{r=r_0} = 0; \quad (5)$$

$$\rho_g (1 - \epsilon) (c_d + ac_g) D \left. \frac{\partial T}{\partial r} \right|_{r=r_0} = Q. \quad (6)$$

In this formulation, the following remain undetermined functions of temperature and porosity: the velocity of the gas phase $w_g(\epsilon)$, the equilibrium degree of adsorption $a(T)$, the heat of adsorption $H(T)$, and the mixing coefficient $D(\epsilon)$. The adsorption rate I , sec^{-1} , is assumed to be large enough so that we can change from Eq. (2) to an equilibrium problem. The above functions are empirical relations. For equilibrium adsorption we took the equations of Dubinin-Astakhov, Bosmadzhan, and van der Waals

$$a(T) = w_0 \rho_m \exp \left[\left(\frac{RT \ln p_s/p}{E} \right)^2 \right], \quad (7)$$

*Equation (1) is solved "from bottom to top," while the other equations are solved "from top to bottom."

TABLE 1. Values of the Initial Data for Computer Calculation

Adsorption system	T_0	$a_0, \%$	ϵ_0	$G_2, \text{kg}/\text{m}^2 \cdot \text{sec}$	r_0, m	R_0, m	$Q, \text{W}/\text{m}^2$
CaA + CO ₂	293	13	0,4	2,2	$8 \cdot 10^{-3}$	$25,5 \cdot 10^{-3}$	$10 \cdot 10^3$
CaA + CO ₂	293	13	0,4	6,0	$8 \cdot 10^{-3}$	$25,5 \cdot 10^{-3}$	$20 \cdot 10^3$

$$\rho_m = \left. \frac{\partial \rho_l}{\partial T} \right|_{T=293\text{K}} (T-293), \quad (8)$$

in which the derivatives of the density of the liquid phase is present

$$p_s = p_{cr} \exp \left(\frac{T - T_{cr}}{T} \frac{H}{RT} \right). \quad (9)$$

We determined the heat of adsorption from the Clapeyron-Clausius equation

$$H(T) = R \left(\frac{\partial \ln p}{\partial \frac{1}{T}} \right) \Big|_{a = \text{const}} \quad (10)$$

The velocity of the gas phase was found from the porosity by means of the Todes equation. However, there is the implicit assumption that the equation is valid for the local mean gas velocity when porosity changes from point to point

$$\omega_g = \frac{v_g}{d_d} \frac{\text{Ar} \epsilon^{4,75}}{18 + 0,6 \sqrt{\text{Ar} \epsilon^{4,75}}}. \quad (11)$$

Finally, we determine the mixing coefficient from the equation [2]

$$D = \begin{cases} 0,013(\omega - \omega_0) X_0 \left(\frac{\sqrt{\frac{4 Y_0 Z_0}{\pi}}}{X} \right)^{0,5} \left(\frac{\omega - \omega_0}{gX} \right)^{-0,15} & \text{at } \epsilon \geq 0,5; \\ 0,94 \frac{1 + 0,807 \cdot 10^{-2}(T - 273)}{(c_d + ac_g)(1 - \epsilon) \rho_d} \lg \frac{0,74 - 0,31(1 - \epsilon_0)}{0,74 - (1 - \epsilon_0)} & \text{at } \epsilon \leq 0,5. \end{cases} \quad (12)$$

In formulating (1), we assumed that the mixing coefficients for the solid and liquid phases were equal (the particle volume diffuses in the same manner as the gas volume). The gas phase is mixed as a result of mixing of the solid phase. This process is analogous to electron-hole conduction seen in semiconductors. The mixing consists of a series of displacements of solid particles and gas. When a particle changes position, its place is taken by gas.

The longitudinal component of mixing is not considered because the vertical gradients are an order smaller than the horizontal gradients in a fluidized bed in a unit with a vertically heated tube. The dominant role in transport processes is played not by longitudinal mixing, but by vertical convective flows of the gas and solid phases. Also, several calculations were performed on a model which considered lengthwise mixing. The model consisted of three elliptical equations with a convective term and was realized on an ES computer. The difference scheme was solved by Fedorenko's method, which speeds up the convergence of the solution of such equations by a factor of more than two. However, the solution of one variant on the ES-1022 computer lasted about 90 min. Such computing time makes the use of the programs infeasible for engineering practice. A series of calculations showed that it is not expedient to introduce the longitudinal components of mixing into the mathematical model of a thermofluidized bed, since it gives a correction no greater than 5% [3].

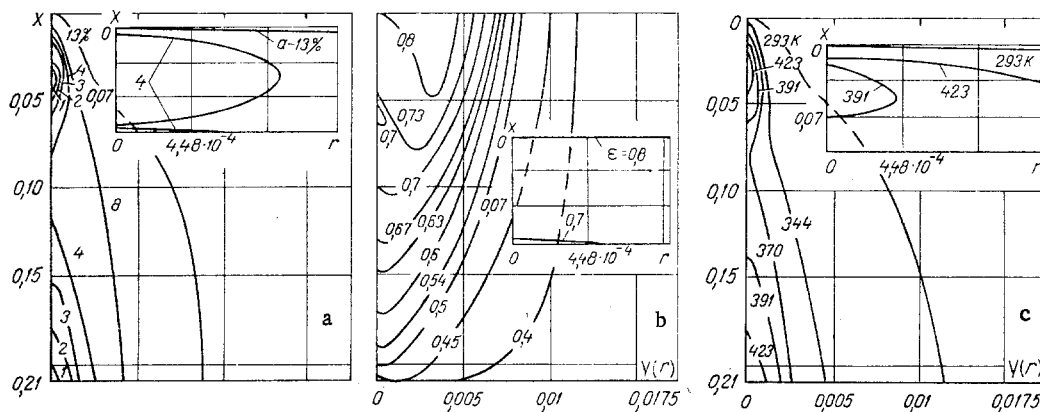


Fig. 3. Change in the degree of adsorption (a), porosity (b), and temperature (c) of the thermofluidized bed: $d = 0.150 \cdot 10^{-3}$ m; $G = 6.0$ kg/m²·sec; $r_a = 0.0175$ m; $Q = 20 \cdot 10^3$ W/m². $X, Y(r), r, m$.

The desorption rate was taken to be proportional to the deviation of the actual degree of adsorption at a given point from the equilibrium value determined by the temperature at that point. The pressure of the sorbate was assumed to be constant in the volume of the system.

With allowance for the above assumptions, Eqs. (1)-(12) constitute a closed system which can be solved numerically by trial run with recalculation of the coefficients.

To substantiate the adequacy of the above model in relation to the actual process, an experiment [4] was conducted on an adsorption-desorption unit to extract carbon dioxide from flue gases. As the sorbent we used CaA zeolite with a mean grain size of $0.2 \cdot 10^{-3}$ m. The desorber for thermal regeneration of the zeolite was a vertical bundle of cylindrical heaters with a diameter of 0.012 m (the spacing of the axes of the heaters was 0.0295 m) and a height of 0.4 m. The equivalent radius of the cylinder R_0 for the mathematical model was found from a section in one heater. The space in the tube bundle of the desorber was filled with spherical packing with a diameter of 0.011-0.013 m.

In the experiments, we varied the degree of adsorption of carbon dioxide at the inlet of the unit and the mean temperature of the heater wall, the length of the tube bundle, and the rate of zeolite flow through the desorber. We measured the temperature of the zeolite and the residual degree of adsorption at the outlet of the unit ($a_0 - a_{x_0} = \Delta a$) and the heat flux from the tubular heaters. The zeolite temperature T_0 at the desorber inlet was kept constant.

The above parameters were monitored as follows. Temperature was measured with Chromel-Alumel thermocouples located at the desorber inlet and outlet and along the heater on its wall. The measurements were accurate to within $\pm 5\%$. The degree of adsorption was measured by probes in the top and bottom sections. This quantity was measured by the gravimetric method to within $\pm 0.1\%$. Heat flux was determined to within $\pm 2.5\%$ from the total power of the electric heaters.

The results of the experiments are shown in Fig. 2, where the curves represent theoretical values. It must be noted that agreement was obtained between the theoretical and experimental data only with the assumption that the desorption rate was finite, with a rate constant I [Eqs. (1)-(3)].

Figure 3 shows isolines of the degree of adsorption, porosity, and temperature for a zeolite flow in the case of a limiting degree of carbon dioxide adsorption. The initial data for the calculation are shown in Table 1. It is evident from the figure that with moderate heating rates and low solid-phase flow rates, gas evolution occurs mainly near the heated wall. Intensive fluidization occurs in the top part of the unit, while a nearly solid layer of sorbent flows in the bottom third of the unit ($\epsilon = 0.5$).

The isolines of temperature and degree of adsorption are regular in character. The peak of gas evolution moves away from the wall and into the flow only in the bottom part of the unit. A different pattern is seen at high flow rates and high heating rates. The flow is fairly intensively fluidized in the top part of the unit, and heat transfer is impeded by thinning of the flow. Here, a zone of overheating of the material is seen on the wall. The

flow interacts most intensively with the wall in the middle and is compacted in the bottom part of the unit.

The calculations show that thermofluidization of a sorbent flow in a desorber improves heating uniformity and increases the degree of regeneration by 20-30% compared to regeneration in a dense flow [1, 3].

NOTATION

T, temperature; a , degree of adsorption, kg/kg; ϵ , porosity; ρ , density; D, mixing coefficient; G, zeolite flow rate in the unit; d, particle diameter; I, desorption rate; c, heat capacity; H, differential heat of adsorption (desorption); w, fluidization velocity; ν , viscosity; p, pressure; Ar, Archimedes number; Q, heat flux. Indices: g, gas phase; d, solid phase; 0, limiting value; a , ϵ , and T, for transport of sorbed and desorbed phases and energy (enthalpy), respectively; wa, wall; m, λ , medium and liquid phase; s, saturated state of sorbate.

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EFFECTIVE TRANSPORT COEFFICIENTS OF TEXTURED MATERIALS

E. A. Mityushov, P. V. Gel'd, R. A. Adamesku,
and A. M. Brynskikh

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A method is proposed for calculating effective transport coefficients of two-phase anisotropic polycrystalline materials with an arbitrary distribution of anisotropic ellipsoidal particles of the first phase.

As is known, anisotropy of the kinetic properties of polycrystalline materials may be due to both crystallographic and mechanical texture. Methods of calculating the effective transport coefficients in such systems have been fairly well developed by now mainly only for isotropic objects [1]. However, anisotropic materials are most often encountered in practice, which makes it necessary to develop methods to evaluate their effective properties.

To solve this problem, first we examine the effect of crystallographic texture on characteristics of a single-phase polycrystalline material. We henceforth assume that there is perfect contact between the phase components (grains, inclusions), i.e., there are no intergranular layers or foreign phases to complicate the description of transport processes. Due to the isotropy of the kinetic properties of polycrystals with a cubic lattice, we will take the symmetry of the structure below to be cubic.

The simplest method of evaluating effective kinetic properties is to average the transport coefficients in individual crystallites for a set of orientations. This approach corres-