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Mathematical simulators for fluidized bed apparatus to study thermochemical processes

TEXT: Equations for the rates of adsorption, desorption, and reaction are derived for the heterogeneous chemical reaction in a fluidized bed: 
\[ a_1A_1 + a_2A_2 = a_3A_3 + a_4A_4 \] 
where \( A_1 \) is the solid, and \( A_2 \) is the gaseous initial substance, \( A_3 \) is the solid and \( A_4 \) the gaseous reaction product, and \( a_1, a_2, a_3, \) and \( a_4 \) are the stoichiometric coefficients.

\[ v_a = C_2^F \sum_{i=1}^{n} K_1^O \cdot \theta_j \cdot \exp \left[ -(E_1^O + \sum_{j} \eta_{A_j} \cdot \theta_{A_j})/RT \right] \] (11) holds for the adsorption rate of \( A_2 \) with respect to unit surface, \( C_2^F \) is the concentration of \( A_2 \), and \( \theta_j \) is a factor having the dimension \( m^3/\text{sec} \); \( E_1^O \) is the activation energy of the free surface; \( \eta_{A_j} = \alpha_j \cdot b \cdot C_{A_j}^{s_{\infty}} \), where \( \alpha \) is the change of energy due to adsorption, \( b \) is a coefficient, and \( C_{A_j}^{s_{\infty}} \) is the concentration of the adsorption centers per unit of surface; \( \theta_{A_j} = C_{A_j}^{s_j}/C_{A_j}^{s_{\infty}} \) is the degree of surface occupation by the substance \( A_j \), with \( C_{A_j}^{s_j} \) being the surface concentration of \( A_j \).

\[ v_{d1} = \frac{1}{\sum_{i=1}^{n} K_{d1}^O \cdot \theta_{A_2j} \cdot \exp \left[ -(E_{d1}^O + \sum_{j} \eta_{A_j} \cdot \theta_{A_j})/RT \right] } \] (17) holds for the desorption rate of \( A_2 \) per unit surface. \( v_r = \sum_{i=1}^{n} K_{ri}^O \cdot \theta_{A_2i} \cdot \exp(-E_{ri}/RT) \) (22) holds for the total rate of the chemical reaction. 

\[ d\theta_{A_2}/dt = v_a - v_d - v_r \]

wherein the values from equations (11), (17), and (22) are to be substituted, holds for the material balance. For the substance \( A_4 \), the concentration of \( A_2 \) on the active surface \( (m^{-3}) \); \( K_1^O \) is a factor having the dimension \( m^3/\text{sec} \); \( E_1^O \) is the activation energy of the free surface; \( \eta_{A_j} = \alpha_j \cdot b \cdot C_{A_j}^{s_{\infty}} \), where \( \alpha \) is the change of energy due to adsorption, \( b \) is a coefficient, and \( C_{A_j}^{s_{\infty}} \) is the concentration of the adsorption centers per unit of surface; \( \theta_{A_j} = C_{A_j}^{s_j}/C_{A_j}^{s_{\infty}} \) is the degree of surface occupation by the substance \( A_j \), with \( C_{A_j}^{s_j} \) being the surface concentration of \( A_j \).
Mathematical simulators for ... B101/B186

Mathematical simulators for adsorption, desorption, and material balance are set up in the same way. The functional diagram of the simulator (Fig. 1) correctly reproduces the course of the heterogeneous thermochemical processes, when the adsorption of $A_2$, the desorption of the reaction product, or the chemical reaction on the active surface are the limiting stages. There are 2 figures.

Fig. 1: Functional diagram of the mathematical simulator for adsorption, desorption, and surface reaction of a heterogeneous process. Legend: $\alpha = a$ = adsorption; $\delta = d$ = desorption; $\rho = r$ = reaction.

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