**Adsorption of Active Trace Gases by Ensemble of Ultrafine Porous Particles with Impermeable Core.**

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**Highlights**

* Originalmodel of gas adsorption by particles with non-uniform porosity is proposed.
* Effect of radioactive decay and kinetic effects on the rate of gas adsorption is studied.
* Gas adsorption by ensemble of particles is governed by integro-differential equation.
* Theoretical predictions are in good agreement with experimental results.

**1. Introduction**

Consider adsorption of atmospheric trace gas from a mixture with inert gas by a moving ensemble of porous particles. The size of the particles can be of the same order of magnitude as mean free path of molecules in air at normal conditions. The velocity of particles is equal to a gas velocity. At time t = 0 particles begin to adsorb active gas from the gaseous mixture. Gas adsorption inside a porous particle is determined by nonstationary equation of diffusion in spherical coordinates with a sink term. Equation of diffusion is supplemented by initial and boundary conditions – zero mass flux at a surface of impermeable core and to be determined from equation of mass balance for a unit cell time-dependent mass flux at gas-particle interface.

**2. Methods**

When the size of a particle have the same order of magnitude as a mean free path, the Fickian diffusion approach for the analysis of reactant molecules transport is not applicable. We overcome this difficulty applying the flux-matching theory (see [1]-[2]) which is a hybridization of the diffusion and the free molecule approaches. The concentration profile of radioactive gas far away from the particle is described by the diffusion equation. This profile coincides with the real one down to the distances of the order of the mean free path of molecules of adsorbate. A limiting sphere is then introduced inside of which the free molecule kinetics governs the adsorbate transport. Then the radius of the limiting sphere is obtained from the condition of equality of the fluxes in both zones.

**3. Results and discussion**

The developed model of radioactive gas adsorption by ultrafine porous particles is applied to investigation of scavenging of radioactive gases from a mixture with air by an ensemble of moving carbon-based aerosols. The results of calculations of concentration of I-132 gas in a gaseous phase as a function of time are shown in Figure 1. Calculations are performed for aerosol number density , the specific surface area of a particle was assumed to be equal to 100, and density of porous particle with radius a=50 nm is 1 . Analysis of Fig. 1 shows that concentration of radioactive trace gas decreases rapidly at the initial stage of gas adsorption. Rapidly decreasing segment of the temporal dependence of concentration is followed by a shallow-slope segment. For large time the concentration of a radioactive trace gas vanishes due to radioactive decay. The slope of the curve at the steep-slope segment of the temporal dependence of concentration increases with an increase of Knudsen number. The magnitude of concentration at a shallow-slope segment of the curve decreases with a decrease of a Knudsen number. The larger the Knudsen number, the larger is a period of time required for concentration of active trace gas in a gaseous phase to reach a shallow-slope segment of the temporal dependence of concentration.



**Figure 1.** Concentration of active gas in a gaseous phase as a function of time.

**4. Conclusions**

We developed a model for adsorption of active atmospheric gases by an ensemble of solid porous particles taking into account radioactive decay in the dispersed and continuous phases. Using the developed model we calculated temporal dependences of concentration of adsorbed gas in a particle, concentration of radioactive gas in a gaseous phase and scavenging coefficient for adsorption of I-131, I-132, Rn-220 and Rn-222 by carbon-based aerosols. The obtained results can be summarized as follows:

1. Mass flux density at the particle interface is determined by integral equation while temporal evolution of concentration of an active trace gas in a gaseous phase is described by integro-differential equation.

2. Neglecting kinetic effects during gas adsorption by ultrafine particles leads to the overestimation of the rate of adsorption.

3. The developed model of radioactive gas scavenging by an ensemble of aerosols yields the same estimate of the dependence of the adsorbed amount of gaseous radioactive Iodine-131 in a particle vs. time as the measurements of Noguchi et al. [3].

**References**

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