Effect of Diffusion Interactions between Droplets on Gas Absorption of Highly Soluble Gases in Sprays and Clusters

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Abstract

Industrial and naturally occurring absorption air pollutants removal processes include wet removal of moderately and highly soluble gases by dispersed liquid phase in various types of packed and spray towers and in-cloud scavenging of highly soluble gases. In this connection the study of gas absorption by clusters of droplets is of great interest for environmental and chemical engineering.

In this study we describe a method that takes into account diffusion interactions between droplets caused by the overlap of the depleted of soluble gas regions around the neighboring droplets. The suggested method employs a cellular model of a gas-droplet suspension whereby a suspension is viewed as a periodic structure consisting of the identical spherical cells with periodic boundary conditions at the cell boundary. It is assumed that gas absorption by cluster of droplets is accompanied by the subsequent aqueous-phase equilibrium dissociation reaction. We showed that scavenging of highly soluble trace gas in a cluster of droplets is described by a system of transient diffusion equations with the corresponding initial and boundary conditions at the droplet center, droplet surface and at the boundary of the cell. The initial boundary value problem was solved using the method of lines and Monte Carlo simulations. Using the proposed model we determined temporal and spatial dependencies of the concentration of the soluble trace gas in a gaseous phase and in a droplet and calculated the rate of gas absorption. It is showed that absorption of highly soluble gases by clusters of droplets leads to a significant decrease of soluble trace gas concentration in the interstitial gas. We found that scavenging coefficient for gas absorption by cloud droplets remains constant and sharply decreases only at the final stage of absorption. This assertion implies the exponential time decay of the average concentration of the soluble trace gas in the gaseous phase and can be used for the parameterization of gas scavenging by cloud droplets in the atmospheric transport modeling.

In the calculations we employed gamma size distributions of droplets. We performed our calculations for several soluble gases such as hydrogen peroxide (H_2O_2) and nitric acid (HNO_3). It was shown that despite of the comparable values of Henry's law constants for the hydrogen peroxide and the nitric acid, the nitric acid is absorbed more effectively by cluster of droplets than the hydrogen peroxide due to a major affect of the dissociation reaction on nitric acid scavenging. We obtained also the analytical expressions for the "equilibrium values" of concentration of the active gas in a gaseous phase and for the total concentration in the liquid phase for the case of the hydrogen peroxide and nitric acid absorption by cloud droplets.

The results of the present study can be useful in an analysis of different meteorology-chemistry models and in particular in various parameterizations of the in-cloud scavenging of the atmospheric soluble gases. Analysis of the diffusion interaction between droplets in stagnant clusters provides a fundamental knowledge of the processes that occur in atomization and spray systems.

The developed cell model of highly soluble gases absorption or parameterizations based on the obtained results can be easily integrated into online coupled meteorology-chemistry or climate-chemistry models, where the cloud processes and chemical transformation of atmospheric pollutants are considered together with two-way interactions as well as it can be used for the modeling of gas absorption by mist formed in gas streams inside various types of packed and spray towers.

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