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Nonlinear dynamics of concentrations for heterogeneous chemical reactions in distributed aerosol systems

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Contemporary atmospheric models usually involve cycles of gas-phase reactions as well as heterogeneous chemical reactions with liquid or solid aerosols. Homogeneous reactions are relatively well studied, but the development of theory of heterogeneous reactions is still in progress.

The distribution and dynamics of concentrations in the atmosphereis subject of description by chemical transport models. These models are important for many environmental applications, especially for distribution of pollutants in the atmosphere or e.g. for destruction of ozone layer. The latter example involves heterogeneous chemical reactions.

A new approach to heterogeneous chemical reactions, that take place at the surface of aerosol particles has been proposed earlier by P. Mchedlov-Petrossyan, W. Zimmerman and G. Khomenko in chemical engineering context and applied to heterogeneous processes in the polar stratospheric clouds. Here we extended this approach onto consecutive chemical reactions. We reveal that the complex spatial distribution of reactants and localisation of maximum production rates appears in aerosol clouds for the system of interacting heterogeneous reactions.

Here we describe the theoretical approach based on the well founded basic primitive hydrodynamic equation as well as concept of local and bulk concentrations and mass-action law and stoichiometric constrains.

A heterogeneous chemical reaction, in contrast to homogeneous one takes place on the surface of the particles while the gas-phase reaction passes in the bulk of fluid, thus the concentration of reactants and the reaction products near the surface of aerosol particles is different from the bulk concentrations. The local concentration is an average value of the surface concentrations over ensemble of aerosol particles. The bulk and local concentrations are macroscopic variables. The formulation of the problem involves advection-diffusion equations with source/sink reaction terms and the algebraic constraints coming from chemical kinetics. This system is strongly non-linear.

We solved the problem numerically and also have found analytical solutions for several limiting cases. The system undergoing consecutive chemical reactions manifests complex spatial distribution of concentrations for different important regimes. We anticipate that the proposed approach yields deeper insight into heterogeneous chemistry and its applications.