Transport properties in chemically reactive mixtures of dilute gases

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The description and modelling of chemically reactive gases is a topic of great interest due to several engineering applications. In particular, the investigation of transport processes and non-equilibrium regimes within physical and chemical systems is fundamental in many industrial applications developed by chemical engineers [1].

The theoretical analysis of the transport processes and non-equilibrium regimes in chemically reactive mixtures can be conducted using the Boltzmann equation (BE) if a kinetic model extending the BE to chemically reactive systems is used.

Here we consider a dilute reactive mixture of four constituents undergoing a reversible chemical reaction of bimolecular type. The mixture is described by the simple reacting spheres (SRS) kinetic model developed by Xystris, Dahler and Qin in a series of papers published in the seventies and nineties of the past century, see, for example, Refs. [2,3].

The SRS model treats both elastic and reactive collisions as hard spheres type and the molecules behave as if they were single mass points with two internal states. Collisions may alter the internal states and this occurs when the kinetic energy of the colliding pair exceeds the activation energy of the molecules. The microscopic reversibility (detailed balance) reduces to a simple condition and all mathematical aspects of the model can be fully justified [4]. Moreover a correction term is introduced in the elastic operator in order to prevent double counting of the events in the collisional integrals.

In the present work we use the Chapman-Enskog method, at the first-order level of the Enskog expansion, to determine the non-equilibrium solution to the SRS kinetic system. The chemical regime is such that both elastic and reactive collisions occur with comparable characteristic times. In this case, the elastic and the reactive source terms in the kinetic equations account for comparable processes and the chemical reaction can be considered in its final stage, close to chemical equilibrium (fast process).

We determine the transport coefficients associated to the chemical reaction rate and shear viscosity and investigate how they are influenced by the chemical reaction and by the "correction" term proper of the SRS model. Some comparisons with results obtained with other models available in literature [5] are also presented.

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