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Transport coefficients for the simple reacting spheres kinetic model I: Reaction rate and shear viscosity

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HIGHLIGHTS

- Transport coefficients for a simple reacting spheres model.
- Influence of the chemical reaction on the transport coefficients.
- Impact of model parameters on the transport coefficients.

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ABSTRACT

In this work, we consider a dilute reactive mixture of four constituents undergoing the reversible reaction $A + B \rightleftharpoons C + D$. The mixture is described by the Simple Reacting Spheres (SRS) kinetic model which treats both elastic and reactive collisions as hard spheres type and introduces a "correction" term in the elastic operator in order to prevent double counting of the events in the collisional integrals. We use the Chapman–Enskog method, at the first-order level of the Enskog expansion, to determine the non-equilibrium solution to the SRS system in a chemical regime for which both elastic and reactive collisions occur with comparable characteristic times. We then determine the transport coefficients and focus our analysis on the evaluation of those coefficients associated with the reaction rate and the shear viscosity. Our numerical evaluation of the transport coefficients allows for the investigation of their behaviour in a suitably chosen parametric space with an opportunity to check how these coefficients are influenced by the chemical reaction and by the "correction" term proper of the SRS model.

1. Introduction

Non-equilibrium effects and transport properties of chemically reactive mixtures are widely investigated in modern fluid dynamics, due to several applications of multicomponent reactive systems in chemical engineering, biotechnology, combustion engineering, propulsion devices and other industrial processes. The description of the chemical kinetics of the reaction mechanism is an important part of the investigation and the application of mathematical models can provide some additional tools to better understand the chemical process [1].

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At this level, the kinetic theory of chemically reactive mixtures improves the knowledge of the reaction dynamics and provides the expressions for the reaction rates of the chemical species [2–4]. There are many contributions in this field, after the pioneering works by Prigogine, Xhrouet and Mahieu [5,6], Present [7,8], Ludwig and Heil [9], Ross and Mazur [10], and here we quote, for example, papers [11–30] which essentially deal with reaction rates and non-equilibrium effects induced by chemical reactions, as well as transport properties and influence of the chemical reaction on transport coefficients.

Broadly speaking, the above mentioned papers use the molecular description proper of the kinetic theory of gases to deduce explicit expressions for both the reaction rates and the transport coefficients and then investigate in detail the role of the chemical reaction in different processes.

The present paper also arises in this direction, but considers a particular kinetic model for a reactive mixture, namely the simple reacting spheres (SRS) kinetic model, which has been developed by Xystris and Dahler [13] and further advanced by Dahler and Qin [31,32]. In the SRS kinetic model, elastic and reactive collisions are assumed of hard-sphere type and are treated in equal par, contrary to other models that treat the reactive terms as a small perturbation of the elastic ones (see, for example, [5,6,11,12]). Therefore, the SRS model results to be appropriate to investigate processes in which chemical reactions play a relevant role. This is the case of the analysis developed in the present paper.

Furthermore, the kinetic equations of the SRS model includes a "correction" term in the elastic operator in order to describe appropriately the collisional dynamics and prevent double counting of the events in the collisional integrals. In contrast to most kinetic models for chemically reactive mixtures (see, for example, [2,20,21,23,26,27]), the SRS model has built-in the micro-reversibility principle (detailed balance) and its satisfaction can be explicitly verified. Additionally, the SRS kinetic theory, if considered in its general formulation, provides a kinetic system of equations of the revised Enskog type for reactive mixtures and this permits to extend the mathematical approach to moderate dense regimes. For the details on the SRS model, see the original papers [13,31,32] and also the mathematical analysis developed in papers [33–37].

Motivated by the robustness of the SRS model, on one side, and by the interest in the detailed description of the chemical kinetics of reactive processes, on the other side, we plan to develop a research program oriented for the explicit evaluation of the reaction rates and transport coefficients, as well as for the influence of the chemical reaction on the related properties of interest.

In this paper, we start with a simpler case of the SRS model in the dilute gas regime, before considering the more challenging case of the SRS model in dense gas regime, and focus our analysis on the evaluation of the transport coefficients associated to reaction rate and shear viscosity of the reactive mixture.

The SRS model in this work is applied to a quaternary reactive mixture of monatomic gases, whose constituents undergo the reversible reaction of bimolecular type. We use the Chapman–Enskog method and the second approximation of the Enskog expansion, to determine the non-equilibrium solution to the SRS system in a chemical regime of fast chemical reaction for which both elastic and reactive collisions occur with comparable characteristic times. We then determine the transport coefficients and investigate the influence of the chemical reaction on such coefficients. We also analyse the impact of the elastic correction term proper of the SRS model on the transport properties.

The paper is organized as follows. In Section 2, we briefly describe the SRS model, with emphasis on the kinetic system, equilibrium properties and macroscopic equations for the hydrodynamic fields. In Section 3, we present the transport algorithm based on the Chapman–Enskog method to obtain the second approximate solution (or the first-order solution) to the SRS kinetic equations. Then, in Section 4, we explicitly derive the linear integral equations for the determination of the transport coefficients associated to the reaction rate and shear viscosity. In Section 5, we implement numerically the transport algorithm presented in Section 3 and use the integral equations derived in Section 4 to evaluate the coefficients of the reaction rate and shear viscosity. We perform many numerical computations in a broadly varying parametric space in order to analyse the influence of the chemical reaction on the behaviour of the transport coefficients. We also investigate the impact of the elastic correction term of the SRS model on the transport coefficients. Finally, in Section 6 we summarize our results and present the final remarks.

2. The SRS kinetic model

In this section we briefly describe the SRS kinetic model for a dilute reactive mixture. For a detailed description, see, for example, [35–37] and the references cited therein.

We consider a four component mixture A, B, C, D whose particles behave as if they were single mass points. Internal degrees of freedom for the gas particles, such as vibrational and rotational energies, are not taken into account. Particles undergo binary elastic collisions and reactive encounters according to a reversible chemical reaction of bimolecular type,

$$A + B \rightleftharpoons C + D. \tag{1}$$

We use the indices 1, 2, 3, 4 for the constituents A, B, C, D, respectively. Moreover, we denote by m_i, d_i and E_i the molecular mass, the molecular diameter and the chemical binding energy of each i-constituent, $i = 1, \ldots, 4$. Reactive collisions occur when the reactive particles are separated by a distance $\sigma_{12} = \frac{1}{2}(d_1 + d_2)$ or $\sigma_{34} = \frac{1}{2}(d_3 + d_4)$, and result in a redistribution of masses and in a rearrangement of energies (kinetic and binding) among the constituents. In particular, the conservation of mass during chemical reactions, see (1), implies that

$$m_1 + m_2 = m_3 + m_4 = M. \tag{2}$$