Reaction diffusion limit of a kinetic model for chemically reactive gas mixtures

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Within the kinetic theory for chemically reactive gases, we consider the simple reacting spheres model for a mixture of four monatomic gases participating in a reversible chemical reaction of bimolecular type. Collisions between the species are either elastic or reactive and are both of hard sphere type. At the macroscopic level, one can describe how the concentration of the species in the reactive mixture changes under the influence of two processes, namely: diffusion, which causes the species to spread in space, and chemical reaction, which results in the transformation of the species into each other. Since the Boltzmann equation can in principle be used to describe convective phenomena, to achieve the macroscopic description of reaction and diffusion processes, the Boltzmann-type equations for the species in the mixture are scaled in a proper way. In particular, we consider the physical situation in which elastic collisions play the dominant role in the evolution process of the species, while chemical reactions are slow, together with the assumption that the Mach and Knudsen numbers are very small and of the same order of magnitude. Furthermore, we assume that the bulk velocities of the species are small and go to zero in the vanishing Knudsen and Mach numbers limit as well as that Isobaric and isothermal conditions are valid. The macroscopic equations are then obtained from the concentration and momentum balance equations of the species, and both the elastic and the reactive production terms appearing in these equations can be explicitly evaluated using Maxwellian distribution functions centered at the mass average velocity of the species. Such input functions define a state close to thermodynamical equilibrium, but they are able to capture the reaction diffusion effects until the equilibrium is reached. In the limit of vanishing Knudsen and Mach numbers, we formally derive the reaction diffusion equations of Maxwell-Stefan type as the hydrodynamic limit of the Boltzmann-type equations for the species in the chemically reactive gas mixture.

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