New kinetic models of dense reactive and inert mixtures

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I consider the modified simple reacting spheres (MSRS) kinetic model that, in addition to the conservation of energy and momentum, also preserves the angular momentum in the collisional processes. In contrast to the line-of-center models, in the MSRS kinetic models, the microscopic reversibility (detailed balance), is built-in and thus all mathematical aspects of the model can be fully justified. In the MSRS model, the molecules behave as if they were single mass points with two internal states. Collisions may alter the internal states of the molecules, and this occurs when the kinetic energy associated with the reactive motion exceeds the activation energy. Reactive and non-reactive collision events are considered to be hard spheres-like. We consider a four component mixture A, B, C, D, in which the chemical reactions are of the type A+B C+D. I provide fundamental physical and mathematical properties of the MSRS model, concerning the consistency of the model, the entropy inequality for the reactive system, the characterization of the equilibrium solutions, the macroscopic setting of the model and the spatially homogeneous evolution. Moreover, I show that the MSRS kinetic model reduces to the previously considered model simple reacting sphere, if the reduced masses of the reacting pairs are the same before and after collisions.

I also consider stochastic variants for both reactive and inert mixtures. In *Transport coefficients in some stochastic models of the revised Enskog equation*, J. Stat. Phys. 109, 569–590 (2002), Polewczak and Stell developed a new liquid-state kinetic theory for particles with interaction potentials that are continuously varying (such as Lennard-Jones particles and inverse-power-law potentials), rather than discontinuous (such as the hard-sphere or square-well potentials). A stochastic smoothing term that represents a distribution of interaction diameters into the kinetic equation was introduced into the revised Enskog equation. This idea is extended to inert and reactive mixtures.

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