Kinetic theory for chemical reactions without a barrier

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Abstract

In the literature of the Boltzmann equation (BE) extended to chemically reacting gases [1], only few works consider reactive processes without a barrier but the corresponding collision terms are restricted to some particular chemical regimes for which no significant changes are needed at the model level [2]. On the other hand, chemical reactions without a barrier are of great interest in many engineering applications of reactive flows and other processes arising in organic chemistry, chemical physics and biophysics [3, 4]. Accordingly, a new model of the BE for binary reactive mixtures is here proposed with the aim of describing symmetric reversible reactions without a barrier, assuming appropriate reactive cross sections without activation energy and introducing suitable improvements in the elastic and reactive collision terms. The resulting model assures the correct balance equations and law of mass action, as well as good consistency properties for what concerns equilibrium and entropy inequality. Moreover different chemical regimes of slow and fast reactions can be described by means of the proposed model.

This is a joint work with Giselle M. Alves and Gilberto M. Kremer.

Keywords: Kinetic theory; Mathematical modeling of fluids; Chemically reacting mixtures; Reaction effects

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