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A conservative multi-group approach to the Boltzmann equations for reactive gas mixtures

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HIGHLIGHTS

- We consider a quaternary gas mixture undergoing a bimolecular chemical reaction.
- We discuss a reactive kinetic model based on Boltzmann like equations.
- We resort to a probabilistic formulation in terms of collision frequencies and kernels.
- We propose a multi-group approach (speed discretization) with suitable weights.
- We prove that the scheme is conservative at any approximation step.

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ABSTRACT

Starting from a simple kinetic model for a quaternary mixture of gases undergoing a bimolecular chemical reaction, multi-group integro-differential equations are derived for the particle distribution functions of all species. The procedure takes advantage of a suitable probabilistic formulation, based on the underlying collision frequencies and transition probabilities, of the relevant reactive kinetic equations of Boltzmann type. Owing to an appropriate choice of a sufficiently large number of weight functions, it is shown that the proposed multi-group equations are able to fulfil exactly, at any order of approximation, the correct conservation laws that must be inherited from the original kinetic equations, where speed was a continuous variable. Future developments are also discussed.

1. Introduction

Modelling and analysis of gas mixtures constitute very stimulating and challenging problems of practical significance, especially if one wants to account for non-conservative effects like chemical reactions. Indeed we are surrounded by gas mixtures in everyday life. They also play an important role in science and technology. Increasingly better tools for their analysis and numerical simulation are required in order to control and predict their behaviour in different environments and physico-chemical situations. On the other hand gas flows with chemical reactions play a crucial role in several applications of paramount importance, like combustion processes, detonation and deflagration waves, chemical reactors, power generation, and space vehicles.

The matter can be handled in the frame of the continuum theory of fluids [1,2], but of course a kinetic approach is highly desirable, not only for a consistent derivation of the relevant fluid-dynamic equations, but also for a better description and

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a deeper understanding of the underlying problems [3–5]. Work on reactive kinetic equations is in progress, starting from suitable models for chemical reactions and state transitions [6–10] for different types of simple reactions.

The problem that will be addressed here concerns the reversible bimolecular reaction

$$A_1 + A_2 \rightleftarrows A_3 + A_4, \tag{1}$$

starting for simplicity from the simplified reactive kinetic model [6], the so-called Rossani–Spiga model [11], in which non-translational degrees of freedom are neglected. The set of integro-differential Boltzmann-like equations governing the distribution functions f_i making up the distribution vector $\underset{\sim}{f}$ of the considered mixture reads as

$$\frac{\partial f_i}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_i = \sum_{j=1}^{4} Q_{ij}[f_i, f_j] + J_i[\underset{\sim}{f}] \equiv Q_i[\underset{\sim}{f}] \quad i = 1, \ldots, 4 \tag{2}$$

where Q_{ij} is the collision integral for mechanical encounters of the (i, j) pair, and J_i is the net gain by collision for species i in the chemical reaction (i, j, h, k), with admissible sequences (1, 2, 3, 4), (2, 1, 4, 3), (3, 4, 1, 2), (4, 3, 2, 1). They are given by five fold integrals involving the differential cross sections for pair elastic scattering σ_{ij}^E, and the reactive cross sections for the chemical reactions σ_{ij}^R (with $\sigma_{ji}^* = \sigma_{ij}^*$, a star standing for either E or R). Each species is endowed with an energy of chemical bond E_i, and the heat of reaction is given by

$$\Delta E = -\sum_{i=1}^{4} \Lambda_i E_i \qquad \underset{\sim}{\Lambda} = (1, 1, -1, -1) \tag{3}$$

in terms of the stoichiometric coefficients Λ_i. Being only matter of convention, we may always assume $\Delta E > 0$, so that an energetic threshold occurs for the direct reaction in (1). Possible activation energies are included in the cross sections, which account for both possible transitions $(i, j) \to (h, k)$ and $(i, j) \to (k, h)$. We shall set $M = m_1 + m_2 = m_3 + m_4$ for the total mass, $r_i = m_i/M$ for mass fractions, $\mu_{ij} = m_i m_j/M = r_i r_j M$ for reduced masses, and $\delta_{ij} = \sqrt{2\Delta E/\mu_{ij}} > 0$.

The general ith reactive collision integral is given by

$$J_i[\underset{\sim}{f}](\mathbf{v}) = \iint U(g - \Lambda_i\delta_{ij}) g \sigma_{ij}^R(g, \hat{\mathbf{n}}\cdot\hat{\mathbf{n}}') \left[\left(\frac{\mu_{ij}}{\mu_{hk}}\right)^3 f_h\left(\mathbf{v}_{ij}^{hk}\right) f_k\left(\mathbf{w}_{ij}^{hk}\right) - f_i(\mathbf{v}) f_j(\mathbf{w}) \right] d_3\mathbf{w} d_2\hat{\mathbf{n}}' \tag{4}$$

where $g = |\mathbf{v}-\mathbf{w}|$, $\hat{\mathbf{n}} = (\mathbf{v}-\mathbf{w})/g$, and $\mathbf{v}_{ij}^{hk} = r_i\mathbf{v} + r_j\mathbf{w} + r_k g_{ij}^{hk}\hat{\mathbf{n}}'$, $\mathbf{w}_{ij}^{hk} = r_i\mathbf{v} + r_j\mathbf{w} - r_h g_{ij}^{hk}\hat{\mathbf{n}}'$, with $g_{ij}^{hk} = \left[\frac{\mu_{ij}}{\mu_{hk}}(g^2 - \Lambda_i\delta_{ij}^2)\right]^{1/2}$. Here U denotes the unit step function, and it actually introduces a threshold for the collision when $\Lambda_i > 0$. In the ranges allowed for reaction, cross sections σ_{ij}^{hk} are related by the micro-reversibility condition

$$\mu_{ij}^2 g^2 \sigma_{ij}^R(g, \hat{\mathbf{n}}\cdot\hat{\mathbf{n}}') = \mu_{hk}^2 \left(g_{ij}^{hk}\right)^2 \sigma_{hk}^R(g_{ij}^{hk}, \hat{\mathbf{n}}\cdot\hat{\mathbf{n}}'). \tag{5}$$

The elastic collision term Q_{ij} may be considered as a specialization of (4) to the sequence (i, j, i, j), by using the elastic rather than the reactive cross section. In this case thus $\Delta E = 0$, $\mu_{hk} = \mu_{ij}$, $\delta_{ij} = 0$, and $g_{ij}^{hk} = g$.

Collision invariants, namely continuous test functions $\underset{\sim}{\phi}(\mathbf{v})$ satisfying, for any $\underset{\sim}{f}$,

$$\sum_{i=1}^{4} \int \phi_i(\mathbf{v}) Q_i(\mathbf{v}) d_3\mathbf{v} = 0, \tag{6}$$

constitute a seven-dimensional linear space, spanned by the independent scalar vectors

$$\begin{pmatrix}1\\0\\1\\0\end{pmatrix}, \quad \begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad \begin{pmatrix}0\\1\\0\\1\end{pmatrix}, \quad \begin{pmatrix}m_1\mathbf{v}\\m_2\mathbf{v}\\m_3\mathbf{v}\\m_4\mathbf{v}\end{pmatrix}, \quad \begin{pmatrix}\frac{1}{2}m_1 v^2 + E_1\\ \frac{1}{2}m_2 v^2 + E_2\\ \frac{1}{2}m_3 v^2 + E_3\\ \frac{1}{2}m_4 v^2 + E_4\end{pmatrix}. \tag{7}$$

Particle conservation is given by the sum of the first and the third one, mass conservation is recovered by linear combination of the first three multiplied by $m_3, m_1 - m_3, m_2$, respectively. The following three vectors represent momentum conservation, and the last one gives conservation of total (kinetic plus reactive) energy.

A Boltzmann lemma and an H-theorem hold [6,7]. Collision equilibria, defined by

$$Q_i[\underset{\sim}{f}](\mathbf{v}) = 0, \quad \forall\mathbf{v}, \ \forall i \tag{8}$$

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