Kinetic approach to reactive mixtures: theory, modelling and applications

Ana Jacinta Soares

Centre of Mathematics, Department of Mathematics and Applications
University of Minho

e-mail: ajsoares@math.uminho.pt

Abstract

Some recent studies arising in the kinetic theory of chemically reactive mixtures will be revisited here, with the aim of describing some methods and tools of the kinetic theory used to model reactive mixtures and investigate some mathematical and physical problems.

Keywords: Mathematical modelling; Kinetic theory; Chemically reactive systems.

1 INTRODUCTION

The kinetic theory of gases is a branch of statistical mechanics which deals with non-equilibrium dilute gases, i.e. gas systems slightly removed from equilibrium. Instead of following the dynamics of each particle, the kinetic theory approach describes the evolution of the gas system in terms of certain statistical quantities, namely velocity distribution functions, which give information about the distribution of particles in the system as well as the distribution of particle's velocities. One of the main tasks is then to deduce the macroscopic properties of the gas system from the knowledge of the molecular dynamics in terms of the distribution functions and, at the same time, to derive governing equations for these macroscopic properties in the hydrodinamic limits.

Historically, the modern kinetic theory starts with the contributions from August Krönig (1822-1879), Rudolf Clausius (1822-1888), James Maxwell (1831-1879) and Ludwig Boltzmann (1844-1906) and the central result of this theory is attributed to the celebrated Boltzmann equation (BE), derived in 1872, see Ref. [1]. This is an integro-differential equation that describes the evolution of a gas as a system of particles (atoms or molecules) interacting through brief collisions in which momentum and kinetic energy of each particle are modified but the states of intramolecular excitation are not affected.

The Boltzmann equation arises in the description of a wide range of physical problems in Fluid Mechanics, Aerospace Engineering, Plasma Physics, Neutron Transport as well as other problems where chemical reactions, relativistic or quantum effects are relevant. From the mathematical point of view, the Boltzmann equation presents several difficulties, mainly associated to the integral form of the collisional term describing the molecular interactions. In particular a general method for solving the Boltzmann equation does not exist, and only equilibrium (exact) solutions are know. Thus the mathematical analysis of the Boltzmann equation, in particular the properties of the collisonal terms, existence theory and approximate methods of solutions, constitute an interesting research topic in Mathematical Physics.

Available techniques for solving the Boltzmann equation and its variants are based on the approximate methods proposed by David Hilbert (1862-1943) in 1912 and by Sidney Chapman (1888-1970) and David Enskog (1884-1947) around 1916-17. The Hilbert method is a formal tool that obtains approximate solutions of the Boltzmann equation in the form of a power series of a small parameter inversely proportional to the gas density (the Knudsen number). Enskog generalized the Hilbert's idea and introduced a systematic formalism for solving the Boltzmann equation by successive approximations, and Chapman followed the method of Maxwell to determine the transport coefficients of diffusion, viscosity and thermal conductivity. The ideas of Enskog combined with the method of Chapman led to the so called Chapman-Enskog method described in Ref. [2] and then followed by several authors and

extended to more general gas systems.

In this paper, we present a general review of some recent studies arising in the kinetic theory of chemically reactive mixtures, mainly oriented to the modelling of reactive systems, mathematical structure and properties of the governing equations, application to detonation dynamics and existence results.

The studies presented in this paper have been obtained in collaboration with several researchers, cited here in chronological order, Miriam Pandolfi Bianchi (Politecnico di Torino, Italy), Gilberto Medeiros Kremer (Universidade Federal do Paraná, Curitiba, Brazil), Filipe Carvalho (CMAT-UM, Ph.D. Student), Jacek Polewczak (California State University, Northridge, LA, USA).

The paper is organized as follows. The main basic aspects of the kinetic theory are introduced in Section2, with emphasis on the mathematical modelling, consistency properties of the kinetic modelling and connection to hydrodynamics. A particular model for symmetric chemical reaction is introduced in Section 3 and then used in Section 4 to mimic detonation problems. The simple reacting spheres (SRS) model is briefly described in Section 5 and an existence result about the solution of the partial differential equations of the model is presented in Section 6.

2 Kinetic theory background

In kinetic theory of gases, the state of a chemically reactive mixture can be described by the Boltzmann equation. There exist several references on this topic and we quote here the relevant contributions presented in the books [3, 4, 5, 6].

In this section, we introduce the background of the kinetic theory of chemically reactive mixtures necessary to follow the general ideas and results presented in the following sections. We have tried to be as concise as possible in this presentation and do not use so much specialized formalisms. However some notations and nomenclature are needed to introduce the topic and the results.

2.1 Mathematical modelling

The present work is restricted to a dilute reactive mixture consisting of *four* constituents, say A_α, $\alpha = 1, 2, 3, 4$, with molecular masses m_α, diameter d_α and chemical binding energies ε_α. Internal degrees of freedom, like translational, rotational and vibra-

tional molecular motions, are not taken into account. Besides elastic scattering, particles undergo reactive collisions with a reversible bimolecular chemical reaction which can be represented schematically by

$$A_1 + A_2 \rightleftharpoons A_3 + A_4 \tag{1}$$
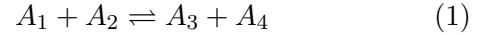
The mass conservation associated to the chemical reaction results in $m_1 + m_2 = m_3 + m_4$. We assume that collisions take place when the particles are separated by a distance $\mathsf{d}_{12} = \frac{1}{2}(\mathsf{d}_1 + \mathsf{d}_2)$ or $d_{34} = \frac{1}{2}(\mathsf{d}_3 + \mathsf{d}_4)$.

A parameter of interest for the present modelling is the heat of the chemical reaction defined as $Q_R = \varepsilon_3 + \varepsilon_4 - \varepsilon_2 - \varepsilon_1$. The chemical reaction is endothermic when $Q_R > 0$ and it is exothermic when $Q_R < 0$.

At the molecular level, the thermodynamic state of the mixture can be described by the constituent distribution functions $f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)$, $\alpha = 1, \ldots, 4$, that represent, at time $t \in \mathbb{R}_0^+$, the number of particles of constituent α with velocity $\boldsymbol{c}_\alpha \in \mathbb{R}^3$ in the point $\boldsymbol{x} \in \mathbb{R}^3$. Functions f_α, $\alpha = 1, \ldots, 4$, are governed, in the phase space, by generalized Boltzmann equations of type

$$\frac{\partial f_\alpha}{\partial t} + \sum_{i=1}^{3} c_i^\alpha \frac{\partial f_\alpha}{\partial \boldsymbol{x}_i} = \mathcal{Q}_\alpha^E + \mathcal{Q}_\alpha^R \tag{2}$$

where the differential term in the left-hand side represents the streaming operator that describes the motion of particles along their trajectories in the phase space, and the term in the right-hand side represents the collision part that describes the changes of particles resulting from collisions. More in detail, $\mathcal{Q}_\alpha^E = \sum_{\beta=1}^{4} \mathcal{Q}_{\alpha\beta}^E$ is the elastic collision term describing the dynamics of inert molecular collisions among constituent α and all other constituents $\beta = 1, \ldots, 4$, and $\mathcal{Q}_\alpha^R$ is the reactive collision term describing the dynamics of chemical interactions. Terms $\mathcal{Q}_\alpha^E$ and $\mathcal{Q}_\alpha^R$ can be written in the following form, see Ref. [6],

$$\mathcal{Q}_\alpha^E = \sum_{\beta=1}^{4} \int_{\mathcal{D} \times \mathbb{R}^3} \left(f_\alpha' f_\beta' - f_\alpha f_\beta \right) g_{\beta\alpha} \sigma_{\beta\alpha} d\Omega_{\beta\alpha} d\mathbf{c}_\beta \tag{3}$$

$$\mathcal{Q}_\alpha^R = \int_{\mathcal{D}^* \times \mathbb{R}^3} \left[f_\beta f_\delta \left(\frac{m_\alpha m_\gamma}{m_\beta m_\delta} \right)^3 - f_\alpha f_\gamma \right] \sigma_{\alpha\gamma}^\star g_{\gamma\alpha} d\Omega^* d\mathbf{c}_\gamma \tag{4}$$

where the primes denote post-collisional states, $g_{\beta\alpha}$ is the relative velocity between the α and β particles, $d\Omega_{\beta\alpha}$ and $d\Omega^*$ are elements of solid angles for elastic and reactive collisional processes,

$\mathcal{D}$ and $\mathcal{D}^*$ the corresponding domains of integration, $\sigma_{\beta\alpha}$ the elastic cross section and $\sigma^*_{\alpha\gamma}$ the reactive cross section. For what concerns the reactive terms, the indices $(\alpha, \gamma, \beta, \delta)$ are from the set $\{(1,2,3,4), (2,1,4,3), (3,4,1,2), (4,3,2,1)\}$.

The specification of the cross sections $\sigma_{\beta\alpha}$ and $\sigma^*_{\alpha\gamma}$ complete the definition of the kinetic model at the molecular level. In general, they satisfy symmetrical relations as those assumed here, of type

$$\sigma_{\beta\alpha} = \sigma_{\alpha\beta}, \quad (m_1 m_2 g_{21})^2 \sigma^*_{12} = (m_3 m_4 g_{43})^2 \sigma^*_{34}$$

In many kinetic theories, $\sigma_{\beta\alpha}$ follows a hard-spheres model, which means that during elastic collisions, the particles behave as if they are rigid spheres, and $\sigma^*_{\alpha\gamma}$ is defined in terms of the activation energy of the chemical reaction, which means that only those particles such that the kinetic energy of the relative motion is greater than the activation energy can collide with chemical reaction.

A kinetic theory based on the statistical description in terms of Eqs. (2) and (3-4) can be of great importance in obtaining a detailed understanding of several processes involving chemically reactive mixtures. The investigation of transport properties and evaluation of transport coefficients is a valuable example. In fact, the transport coefficients of viscosity, diffusion, thermal conductivity and others can not be obtained from macroscopic theories; they have been supplied by experiments and phenomenological considerations. However the kinetic theory can provide these coefficients from the knowledge of the solution of the Boltzmann equation, even if only approximate soloutions are available in general.

2.2 Consistency properties of the kinetic modelling

The kinetic modelling defined in terms of Eqs. (2) and (3-4) possesses the following properties consistent with the chemical kinetics of the reaction, macroscopic laws and equilibrium state.

2.2.1 Proposition (Elastic terms).
The elastic collision terms are such that

$$\int_{\mathbb{R}^3} \mathcal{Q}^E_\alpha \, d\boldsymbol{c}_\alpha = 0, \quad \alpha = 1, \ldots, \alpha \tag{5}$$

that is, elastic collisions do not modify the number of particles of each constituent. □

2.2.2 Proposition (Reactive terms).
The reactive collision terms are such that

$$\int_{\mathbb{R}^3} \mathcal{Q}^R_1 \, d\boldsymbol{c}_\alpha = \int_{\mathbb{R}^3} \mathcal{Q}^R_2 \, d\boldsymbol{c}_\alpha \tag{6}$$

$$= -\int_{\mathbb{R}^3} \mathcal{Q}^R_3 \, d\boldsymbol{c}_\alpha = -\int_{\mathbb{R}^3} \mathcal{Q}^R_4 \, d\boldsymbol{c}_\alpha$$

that is, reactive collisions assure the correct chemical exchange rates for the chemical reaction (1). □

Motivated by the above Proposition 2.2.2, the *reaction rate* of the α-constituent, that gives the production rate of α-particles, is defined by

$$\tau_\alpha = \int_{\mathbb{R}^3} \mathcal{Q}^R_\alpha \, d\boldsymbol{c}_\alpha, \quad \text{with} \quad \tau_1 = \tau_2 = -\tau_3 = -\tau_4 \tag{7}$$

2.2.3 Proposition (Conservation laws).
Elastic and reactive collision terms are such that

$$\sum_{\alpha=1}^4 \int_{\mathbb{R}^3} \Psi_\alpha \mathcal{Q}^E_\alpha \, d\boldsymbol{c}_\alpha = 0 \tag{8}$$

$$\sum_{\alpha=1}^4 \int_{\mathbb{R}^3} \Psi_\alpha \mathcal{Q}^R_\alpha \, d\boldsymbol{c}_\alpha = 0 \tag{9}$$

where $(\Psi_1, \Psi_2, \Psi_3, \Psi_4)$ is a function of the molecular velocities $\boldsymbol{c}_\alpha$ whose components are given alternatively by

$$\Psi_\alpha = m_\alpha$$
$$\Psi_\alpha = m_\alpha \boldsymbol{c}_{\alpha x}, \ \Psi_\alpha = m_\alpha \boldsymbol{c}_{\alpha y}, \ \Psi_\alpha = m_\alpha \boldsymbol{c}_{\alpha z} \tag{10}$$
$$\Psi_\alpha = \frac{1}{2} m_\alpha \boldsymbol{c}^2_\alpha + \varepsilon_\alpha$$

Therefore elastic and reactive collision terms are consistent with the physical conservation laws for mass, momentum components and total energy of the whole mixture. □

2.2.4 Proposition (Equilibrium).
The following conditions are equivalent

(a) $\mathcal{Q}^E_\alpha = 0$ and $\mathcal{Q}^R_\alpha = 0$, $\alpha = 1, \ldots, 4$

(b) $\sum_{\alpha=1}^4 \int_{\mathbb{R}^3} \left(\mathcal{Q}^E_\alpha + \mathcal{Q}^E_\alpha \right) \log\left(\frac{f_\alpha}{m^3_\alpha} \right) d\boldsymbol{c}_\alpha = 0$

(c) f_α is Maxwellian, $f_\alpha = f^M_\alpha$, given by

$$f^M_\alpha = n_\alpha \left(\frac{m_\alpha}{2\pi kT} \right)^{3/2} \exp\left(-\frac{m_\alpha (\boldsymbol{c}_\alpha - \boldsymbol{u})^2}{2kT} \right) \tag{11}$$

3

for $\alpha = 1, \ldots, 4$, where k is the Boltzmann constant, and n_α, $\boldsymbol{u}$, T are functions of $(\boldsymbol{x}, t)$, see Subsection 2.3, with

$$\frac{n_1 n_2}{n_3 n_4} = \exp\left(\frac{Q_R}{kT}\right)\left(\frac{m_1 m_2}{m_3 m_4}\right)^{3/2} \qquad (12)$$

$\square$

Proposition 2.2.4 characterizes Maxwellian distributions defining an equilibrium solution of the Boltzmann Eqs. (2). More in detail, Maxwellian distributions (11) with uncorrelated number densities n_α characterize a mechanical equilibrium only, in the sense that $\mathcal{Q}_\alpha^E = 0$ but $\mathcal{Q}_\alpha^R \neq 0$ in general. Conversely, Maxwellian distributions (11) with the number densities constrained to the mass action law (12) characterize a complete thermodynamical equilibrium state (mechanical and chemical), since $\mathcal{Q}_\alpha^E = 0$ and $\mathcal{Q}_\alpha^R = 0$.

2.2.5 PROPOSITION (ENTROPY PRODUCTION).
Elastic and reactive collision terms are such that

$$-\sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} \log\left(\frac{f_\alpha}{m_\alpha^3}\right) \mathcal{Q}_\alpha^E \, d\boldsymbol{c}_\alpha \geq 0 \qquad (13)$$

$$-\sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} \log\left(\frac{f_\alpha}{m_\alpha^3}\right) \mathcal{Q}_\alpha^R \, d\boldsymbol{c}_\alpha \geq 0 \qquad (14)$$

Moreover, the convex function

$$\mathcal{H}(t) = \sum_{\alpha=1}^{4} \int_{\mathcal{S}} \int_{\mathbb{R}^3} f_\alpha \log\left(\frac{f_\alpha}{m_\alpha^3}\right) d\boldsymbol{c}_\alpha d\boldsymbol{x} \qquad (15)$$

with $\mathcal{S}$ being a closed domain in $\mathbb{R}^3$ where the mixture evolves, is a Liapunov functional for the extended Boltzmann equations (2), that is

- $\dfrac{d\mathcal{H}}{dt}(t) \leq 0$, for $t \geq 0$,

- $\dfrac{d\mathcal{H}}{dt}(t) = 0$, iff the distribution functions are Maxwellian characterized by Eqs. (11-12). $\square$

The first part of Proposition 2.2.5 means that both elastic and reactive collisions contribute to increase the entropy of the mixture. The second part indicates that the $\mathcal{H}$-function drives the reactive mixture from the initial distribution to an equilibrium state.

The proof of the second part of the proposition, see Ref. [7], indicates that function $\mathcal{H}$ splits into a *mechanical* part and a *reactive* part, $\mathcal{H}^E + \mathcal{H}^R$, such

that both $\mathcal{H}^E$ and $\mathcal{H}^R$ show a time decreasing behaviour and that $\frac{d\mathcal{H}^E}{dt} = 0$ iff f_α are Maxwellian given by (11), whereas $\frac{d\mathcal{H}^R}{dt} = 0$ iff f_α are Maxwellian constrained by (12).

2.3 CONNECTION TO HYDRODYNAMICS

The kinetic model previously introduced provides a consistent macroscopic theory in the hydrodynamic limit of Euler or Navier-Stokes level.

2.3.1 Macroscopic variables

The starting point foi the macroscopic description is the definition of certain average quantities, called macroscopic variables, taken over the distributions f_α by integrating with respect to the velocities $\boldsymbol{c}_\alpha$. The number density of each constituent and the one of the mixture are given by

$$n_\alpha(\boldsymbol{x}, t) = \int_{\mathbb{R}^3} f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) \, d\boldsymbol{c}_\alpha, \quad n = \sum_{\alpha=1}^{4} n_\alpha$$

and the corresponding mass densities are defined as

$$\varrho_\alpha(\boldsymbol{x}, t) = m_\alpha \, n_\alpha(\boldsymbol{x}, t), \quad \varrho = \sum_{\alpha=1}^{4} \varrho_\alpha$$

The mean velocity of the mixture is given by

$$\boldsymbol{u}(\boldsymbol{x}, t) = \frac{1}{\varrho(\boldsymbol{x}, t)} \sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} m_\alpha \boldsymbol{c}_\alpha f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) \, d\boldsymbol{c}_\alpha$$

and the diffusion velocity of each constituent is

$$\boldsymbol{u}_\alpha(\boldsymbol{x}, t) = \frac{1}{\varrho_\alpha(\boldsymbol{x}, t)} \int_{\mathbb{R}^3} m_\alpha(\boldsymbol{c}_\alpha - \boldsymbol{u}) f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) \, d\boldsymbol{c}_\alpha$$

The components of the mixture stress tensor are

$$p_{ij}(\boldsymbol{x}, t) = \sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} m_\alpha(\boldsymbol{c}_{\alpha i} - \boldsymbol{u}_i)(\boldsymbol{c}_{\alpha j} - \boldsymbol{u}_j)$$
$$\times f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) \, d\boldsymbol{c}_\alpha$$

The pressure of the mixture is defined by

$$p(\boldsymbol{x}, t) = \frac{1}{3} \sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} m_\alpha(\boldsymbol{c}_\alpha - \boldsymbol{u})^2 f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) \, d\boldsymbol{c}_\alpha$$

so that the temperature is assumed as

$$T(\boldsymbol{x}, t) = \frac{p(\boldsymbol{x}, t)}{kn(\boldsymbol{x}, t)}$$

The components of the heat flux of the mixture are

$$\boldsymbol{q}_i(\boldsymbol{x},t) = \sum_{\alpha=1}^{4} \left(\int_{\mathbb{R}^3} \frac{1}{2} m_\alpha (\boldsymbol{c}_\alpha - \boldsymbol{u})^2 (\boldsymbol{c}_{\alpha i} - \boldsymbol{u}_i) \right.$$

$$\left. \times\, f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)\, d\boldsymbol{c}_\alpha + n_\alpha \varepsilon_\alpha \boldsymbol{u}_{\alpha i} \right)$$

2.3.2 Balance equations

To complete the connection, one can derive the balance equations and the conservation laws describing the balance of the constituent number densities, and conservation of both momentum components and total energy of the whole mixture. It is enough to consider the Boltzmann Eqs. (2), then multiply both sides by the elementary function Φ_α whose components are $\Phi_{\alpha\beta} = \delta_{\alpha\beta}$ and functions (10) of Proposition 2.2.3, and finally integrate with respect to $\boldsymbol{c}_\alpha$. The resulting equations are

$$\frac{\partial n_\alpha}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\big(n_\alpha \boldsymbol{u}_{\alpha i} + n_\alpha \boldsymbol{u}_i\big) = \tau_\alpha \qquad (16)$$

$$\frac{\partial}{\partial t}\big(\varrho \boldsymbol{u}_i\big) + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\big(p_{ij} + \varrho \boldsymbol{u}_i \boldsymbol{u}_j\big) = 0, \ i=1,2,3 \quad (17)$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2} nkT + \sum_{\alpha=1}^{4} n_\alpha \varepsilon_\alpha + \frac{1}{2}\varrho \boldsymbol{u}^2\right) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left[\boldsymbol{q}_i \right. \quad (18)$$

$$\left. + \sum_{j=1}^{3} p_{ij}\boldsymbol{u}_j + \left(\frac{3}{2} nkT + \sum_{\alpha=1}^{4} n_\alpha \varepsilon_\alpha + \frac{1}{2}\varrho \boldsymbol{u}^2\right)\boldsymbol{u}_i \right] = 0$$

Macroscopic Eqs. (16-18) constitute a system of 8 equations in 36 uknowns, namely n_α, τ_α, $\boldsymbol{u}_{\alpha i}$, $\boldsymbol{u}_i$, p_{ij}, T and q_i, where $\alpha = 1,2,3,4$ and $i,j = 1,2,3$. To close the system one passes to the hydrodynamic limit and deduces the constitutive equations for the 28 unknowns τ_α, $\boldsymbol{u}_{\alpha i}$, p_{ij} and q_i.

2.3.3 Hydrodynamic limit

The passage of the kinetic level of Eqs. (2) to the hydrodynamic limit requires the solution of the Boltzmann Eqs. (2), that can be obtained resorting to a systematic expansion technique, see Refs. [2, 5, 6, 8] for a detailed description of the Chapaman-Enskog method, Hilbert method and moment method.

In particular, concerning the Chapaman-Enskog (CE) method, one starts with an appropriate scalling of Eqs. (2) in terms of the so called elastic and reactive Knudsen numbers [3], consistent with the chemical regime of validity of the resulting macroscopic equations. This scaling defines a clear separation of the effects of the *fast* and *slow* processes,

the former being some collisonal processes (elastic or reactive) that drive the distribution function towards a local equilibrium state, and the latter being the other processes that contribute to disturb the distribution function. Then one assumes that the thermodynamical state of the reactive mixture is close to the equilibrium and looks for a solution of Eqs. (2) of type

$$\widetilde{f}_\alpha = f_\alpha^{(0)} \left[1 + \sum_{n=1}^{+\infty} \varepsilon^n \phi_\alpha^{(n)} \right] \qquad (19)$$

where $f_\alpha^{(0)}$ is a quasi-equilibrium distribution function, ε represents a formal expansion parameter related to the Knudsen numbers (then it is settled equal to one) and $\sum_{n=1}^{+\infty} \varepsilon^n \phi_\alpha^{(n)} f_\alpha^{(0)}$ is the disturbance induced by the slow processes, that is assumed to be small.

Introducing expansion (19) into Eqs. (2), neglecting non-linear terms in the disturbances and equating equal terms in ε^n, one obtains linear integral equations for the zero-order term $f_\alpha^{(0)}$ as well as for the disturbances $\phi^{(1)}$, $\phi^{(2)}$, etc. The consistency properties introduced in Subsection 2.2 are fundamental to obtain the solution of these integral equations. After an involved analysis of the equations, the disturbances are obtained as functions of n_α, $\boldsymbol{u}$, T and both transport fluxes and transport coefficients. Inserting the considered approximate solution into the definitions of the reaction rate τ_α, diffusion velocities $\boldsymbol{u}_{\alpha i}$, stress tensor p_{ij} and heat flux q_i, one obtains the constitutive equations that allow to close the macroscopic Eqs. (16-18).

In particular, it comes out that the zero-order approximation $f_\alpha^{(0)}$ is the Maxwellian distribution (11) that leads to the reactive Euler equations without transport effects; the first-order perturbed distributions, $f_\alpha^{(0)}(1 + \phi_\alpha^{(1)})$, are governed by linearized Boltzmann equations and lead to the Navier-Stokes equations involving the transport effects of diffusion, viscosity, thermal conductivity and maybe others; successive approximations lead to the Burnett and super Burnett complicated equations.

According to Propositions 2.2.4 and 2.2.5, one concludes that in a hydrodynamic limit of an Eulerian regime, the *mechanical* entropy of the mixture remains constant and slow reactive processes contribute to drive the mixture from a mechanical to a complete thermodynamical equilibrium state. Conversely, in the hydrodynamic limit associated to the Navier-Stokes equations, both elastic and reactive

collisions contribute to increase the entropy of the mixture, and the entropy flux is also due to diffusion, heat transfer and sheat viscosity phenomenon.

The Chapman-Enskog method converges asymptotically for small Knudsen number, and the Euler and Navier-Stokes equations have a good accuracy.

3 Model for symmetric reaction

A very simple model corresponds to a binary mixture of constituents A and B undergoing the symmetric reaction $A + A \rightleftharpoons B + B$. In this particular case, one has $A_2 = A_1 = A$, $A_4 = A_3 = B$, so that $m_B = m_A = m$, $\mathsf{d}_\alpha = \mathsf{d}$, $\varepsilon_2 = \varepsilon_1 = \varepsilon_A$, $\varepsilon_4 = \varepsilon_3 = \varepsilon_B$, $Q_R = 2(\varepsilon_B - \varepsilon_A)$. Assuming hard sphere cross sections for elastic collisions and step cross sections with activation energy for reactive interactions, the collision terms are (see Ref. [9] for a complete description of the model)

$$\mathcal{Q}_\alpha^E = \sum_{\beta=A}^{B} \int \left(f_\alpha' f_\beta' - f_\alpha f_\beta \right) \mathsf{d}^2 g_{\beta\alpha} \cdot \mathbf{k}_{\beta\alpha} \, d\mathbf{k}_{\beta\alpha} d\mathbf{c}_\beta \quad (20)$$

$$\mathcal{Q}_\alpha^R = \int \left(f_\beta f_\beta' - f_\alpha f_\alpha' \right) \sigma_\alpha^\star g_\alpha \cdot \mathbf{k}_\alpha \, d\mathbf{k}_\alpha d\mathbf{c}'_\alpha \quad (21)$$

In expression (21), the primes are used to distinguish two identical particles that participate in the reactive event, and $\sigma_\alpha^\star$ is given by

$$\sigma_\alpha^\star = \begin{cases} s^2 \mathsf{d}^2 & \text{if} \quad \gamma_\alpha > \varepsilon_\alpha^\star \\ 0 & \text{if} \quad \gamma_\alpha < \varepsilon_\alpha^\star \end{cases} \quad (22)$$

where s represents the steric factor, γ_α is the relative translational energy, $\varepsilon_\alpha^\star$ the forward ($\alpha = A$) and backward ($\alpha = B$) activation energy, both expressed in units of the thermal energy of the mixture, kT,

$$\gamma_\alpha = \frac{m g_\alpha^2}{4kT}, \qquad \varepsilon_\alpha^\star = \frac{\varepsilon_\alpha}{kT}$$

At the macroscopic scale, the mixture is described by the variables n_A, n_B, $\boldsymbol{u}$, T, that are governed by balance equations and conservation laws of type (16) and (17-18). At the hydrodynamic Euler level, and for a chemical regime in which elastic collisions are more frequent than reactive encounters, the Chapman-Enskog method has been used in [9] to obtain the following approximate solution for the distribution function

$$\widetilde{f}_\alpha = f_\alpha^M \left[1 + \phi_\alpha \right], \quad (23)$$

where f_α^M is a Maxwellian distribution and

$$\phi_\alpha = \left(\frac{15}{8} - \frac{5m(c_\alpha - v)^2}{4kT} + \frac{m^2(c_\alpha - v)^4}{8k^2T^2} \right) \quad (24)$$

$$\times x_A^2 \frac{\mathsf{d}^2}{\mathsf{d}_r^2} \frac{Q_R^\star}{8} \left(Q_R^\star + Q_R^\star \varepsilon_A^\star - \varepsilon^\star + 2\varepsilon_A^{\star 2} - 1 \right) e^{-\varepsilon_A^\star}$$

with $x_A = n_A/n$ being the concentration of constituent A, d_r the reactive molecular diameter and $Q_R^\star = Q_R/kT$. Expression (23) indicates that this solution characterizes a non-equilibrium state and expression (24) specifies the deviation from the equilibrium in terms of the activation energy $\varepsilon_A^\star$ and reaction heat $Q_R^\star$. The macroscopic equations associated to this hydrodynamic limit characterizes a non-difusive, non-heat conducting and non-viscous reactive mixture, that is

$$\boldsymbol{u}_{\alpha i} = 0, \qquad \boldsymbol{q}_i = 0, \qquad p_{ij} = p \delta_{ij}$$

and the reaction rate is explicitly given by

$$\tau_B = -\tau_A, \quad \tau_A = -4 n_A^2 \mathsf{d}_r^2 \sqrt{\frac{\pi kT}{m}} \, e^{-\varepsilon_A^\star} \, \Theta \quad (25)$$

$$\Theta = \left[1 + \varepsilon_A^\star + \frac{x_A^2}{128} \left(\frac{\mathsf{d}}{\mathsf{d}_r} \right)^2 Q_R^\star \left(1 + Q_R^\star + Q_R^\star \varepsilon_A^\star \right. \right.$$

$$\left. \left. + \varepsilon_A^\star - 2\varepsilon_A^{\star 2} \right) \left(4\varepsilon_A^{\star 3} - 8\varepsilon_A^{\star 2} - \varepsilon_A^\star - 1 \right) e^{-\varepsilon_A^\star} \right]$$

The hydrodynamic equations are the reactive Euler equations corrected with the effects of the reaction heat. In one space dimension, they are given by

$$\frac{\partial n_\alpha}{\partial t} + \frac{\partial}{\partial x} \left(n_\alpha u \right) = \tau_\alpha, \quad \alpha = A, B \quad (26)$$

$$\frac{\partial u}{\partial t} + \frac{1}{\varrho} \frac{\partial p}{\partial x} + u \frac{\partial u}{\partial x} = 0 \quad (27)$$

$$\frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + \frac{5}{3} p \frac{\partial u}{\partial x} + \frac{2}{3} \sum_{\alpha=A}^{B} \varepsilon_\alpha \tau_\alpha = 0 \quad (28)$$

where u is now the x-component of the mixture velocity.

4 Application to detonation phenomenon

Detonation is a rapid and violent form of combustion accompanied by an important energy release. The propagation of detonation waves in gaseous explosives is a problem of great practical importance, due to the economic impact as well as several engineering applications, such as safety and military issues, propulsion devices and hard rock mining.

A detonation is essentially a reacting wave consisting in a leading shock that propagates into the

explosive, followed by a reaction zone where the reactants transform into products. The shock heats the material by compressing it so that a rapid and violent chemical reaction is triggered.

On the other hand, experimental and computational investigations show that the detonation wave, specially in gaseous mixtures, tends to be unstable to small perturbations and exhibit a significant unsteady structure. The first step of a formal study of the detonation instability is the analysis of the hydrodynamical stability, which consists in imposing small deviations in the steady solution and studying the evolution of the state variables perturbations. The assumption of small deviations allows to linearize the equations and determine the instability modes and growth rate perturbations.

The kinetic theory of chemically reactive mixtures can be used to study the detonation phenomenon and describe some of the physical and chemical aspects observed in experiments. In particular the kinetic modelling of Section 3 has been used in Ref. [10] to investigate the propagation and hydrodynamic stability of a steady detonation wave in a binary reactive mixture with a symmetric chemical reaction. In this section we present the main aspects of this study, with emphasis on the spatial structure of the steady detonation wave and the response of the steady solution to one-dimensional disturbances.

4.1 Dynamics of steady detonation waves

We consider a detonating binary mixture undergoing a reversible reaction of symmetric type, described by the kinetic modelling of Section 3. The mathematical analogue for the detonation dynamics is the hyperbolic set of reactive Euler equations (26-28). Such equations admit steady traveling wave solutions that describe a combustion regime in which a strong planar shock wave ignites the mixture and the burning keeps the shock advancing and proceeding to equilibrium behind the shock. The Zeldovich, von Neumann and Doering (ZND) idealized model [11, 12] gives a good and accepted description of the detonation wave solution. The configuration of the ZND wave consists of a leading, planar, non-reactive shock wave propagating with constant velocity D, followed by a finite reaction zone where the chemical reaction takes place. The spatial structure of the detonation wave is determined by means of the Rankine-Hugoniot conditions, connecting the fluxes

of the macroscopic quantities ahead (superscrip +) and behind (plain symbols) the shock front, together with the rate equation, describing the advancement of the chemical process in the reaction zone. They can be written in the form

$$\frac{dn_A}{dx} = \frac{Dt_c\tau_A}{v - D + n_A\frac{dv}{dn_A}} \qquad (29)$$

$$n_B(n_A) = \frac{(n_B^+ + n_A^+)D}{D - u} - n_A \qquad (30)$$

$$T(n_A) = \frac{(D - u)(\varrho^+ Du + n^+ kT^+)}{n^+ kD} \qquad (31)$$

$$v(n_A) = \frac{2Q_R^* n_A + 3\varrho^+ D^2 - 5n^+ kT^+}{8\varrho^+ D} \qquad (32)$$

$$+ \frac{1}{8\varrho^+ D}\left[\left(2Q_R^* n_A + 3\varrho^+ D^2 - 5n^+ kT^+\right)^2 - 32\varrho^+ Q_R^* D^2 \left(n_A - n_A^+\right)\right]^{1/2}$$

System (29-32), with detonation velocity D, reaction heat Q_R^* and activation energy ε_A^* as parameters, characterize any arbitrary state within the reaction zone (plain symbols) in dependence of the quiescent initial state (superscrip +). This system has been solved numerically with the following input data for kinetic and thermodynamical reference parameters

$$D = 1700\,ms^{-1}, \quad m = 0.01\,Kg/mol,$$
$$E_A = 2400\,K, \quad \varepsilon_A^\star = 6$$
$$T^+ = 298.15\,K, \quad n_A^+ = 0.35\,mol/l, \quad n_B^+ = 0\,mol/l,$$

Some numerical simulations have been performed in Ref. [10] to determine the structure of the detonation wave in both cases of exothermic ($Q_R^* < 0$) and endothermic ($Q_R^* > 0$) chemical reactions. Figures 1 and 2 show representative profiles for the mixture pressure p in both cases of exothermic and endothermic chemical reactions, respectively. The configuration of the solution consists in a reactive rarefaction wave (Figure 1) when the reaction is exothermic and reproduces the typical structure of an idealized ZND wave arising in real explosive system with exothermic chemical reaction [11, 12]. Conversely, the configuration of the solution consists in a reactive compression wave (Figure 2) when the reaction is endothermic and reproduces the essential features of the endothermic stage of a typical chain-branching reactive system with pathological-type detonation [11, 12]. Such detonation occurs when further complexities are introduced in the reactive system and

some dissipative effects are present.
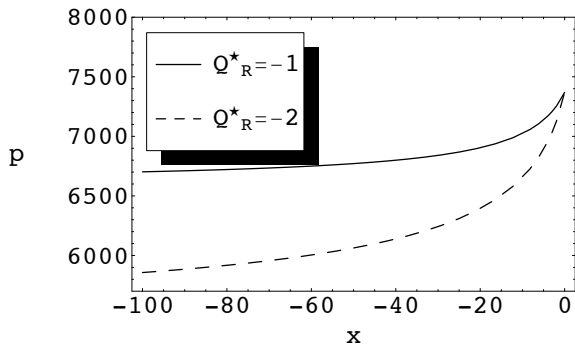
Figure 1. Detonation wave profile (exothermic chemical reaction) for the mixture pressure p.
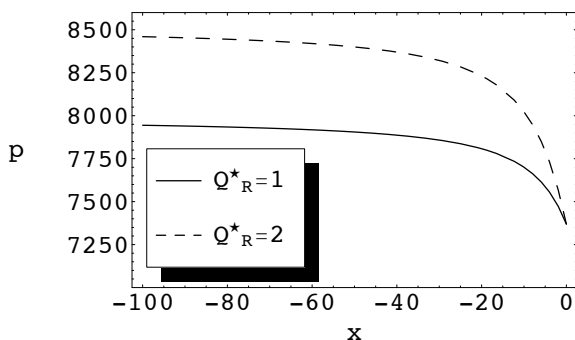
Figure 2. Detonation wave profile (endothermic chemical reaction) for the mixture pressure p.

Other numerical simulations have been considered in Ref. [10] to supplement the representation of the detonation dynamics.

4.2 LINEAR STABILITY OF STEADY DETONATION WAVES

The stability of the steady detonation solution described in Subsection 4.1 is formulated in terms of an initial-boundary value problem describing the evolution of the state variables perturbations.

We assume that a small rear boundary perturbation is assigned so that a distortion in the shock wave position is observed; such distortion induces further perturbations in the state variables and the steady detonation solution can degenerate into an oscillatory solution in the long-time limit.

From the mathematical point of view, the stability problem requires the transformation to the perturbed shock attached frame, and then the linearization of the reactive Euler equations and Rankine-Hugoniot conditions around the steady detonation solution. A normal mode approach with exponential time dependent perturbations and complex growth rate parameter is adopted and standard techniques

are used to deduce the stability equations as well as initial and boundary conditions. The details are omitted here due to the space limitations. The reader is addressed to Ref. [10] and the references therein cited for the a comprehensive study on the detonation satbility.

The initial boundary value problem describing the detonation stability has been numerically treated in Ref. [10], using a rather involved numerical scheme that combines an iterative shooting technique with the argument principle. For a given set of thermodynamical and chemical parameters describing the steady detonation solution, the disturbances of the state variables have been determined in a given rectangular domain of the growth rate parameter. and detailed information about the instability parameter regimes have been provided.

Figure 3 represents the stability boundary in the parameter plane defined by the reaction heat Q_R^* and forward activation energy $\varepsilon_A^\star$.
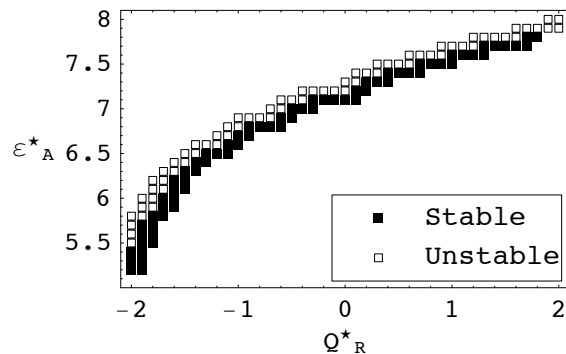
Figure 3. Stability boundary in the $Q_R^* - \varepsilon_A^*$ plane.

In this representation, a pair $(Q_R^*, \varepsilon_A^\star)$ in the stability zone indicates that for the corresponding values of the reaction heat and activation energy, no instability modes have been found. Conversely, a pair in the instability zone indicates that for the corresponding values of the reaction heat and activation energy, one instability mode, at least, has been found. Moreover, Figure 3 reveals that for a fixed value of the activation energy, the detonation becomes stable for larger values of the reaction heat, whereas for a fixed value of the reaction heat, the detonation becomes stable for smaller values of the activation energy. These results are consistent with known experimental works and numerical simulations [12], in the sense that increasing the reaction heat, or decreasing the activation energy, tends to stabilize the detonation.

5 SIMPLE REACTING SPHERES MODEL

The simple reacting spheres model considers hard-sphere cross sections for elastic collisions and reactive cross sections with activation energy, of hard-spheres type. The molecules behave as if they were single mass points with two internal states of excitation. Collisions may alter the internal states and this occurs when the kinetic energy associated with the reactive motion exceeds the activation energy.

The kinetic theory of simple reacting spheres (SRS) has been developed in Ref. [13] for a quaternary mixture A, B, C, D with the assumptions of no mass exchange ($m_1 = m_3$, $m_2 = m_4$) and no alteration of particle diameters ($\mathsf{d}_1 = \mathsf{d}_3$, $\mathsf{d}_2 = \mathsf{d}_4$). Further advances concerning essentially physical and mathematical properties of the SRS sytem and existence theory for the partial differential equations of the model have been considered in Refs. [14, 15, 16, 17]. The SRS theory has been extended in Ref. [18], with no restrictions on the molecular masses and diameters, and a global existence result has been stated.

The SRS modelling refers to the reactive mixture introduced in Section 2, whose particles undergo the reversible bimolecular reaction (1). The reactive Boltzmann equations for this mixture have the general form of Eqs. (2) but the collisional terms are corrected for the occurrence of reactive encounters. More specifically, the elastic operator contains a correction term which subtracts from the total number of collisions those events that lead to chemical reaction. As before, we assume that collisions take place when the particles are separated by a distance $\mathsf{d}_{12} = \frac{1}{2}(\mathsf{d}_1 + \mathsf{d}_2)$ or $\mathsf{d}_{34} = \frac{1}{2}(\mathsf{d}_3 + \mathsf{d}_4)$, but only those particles such that the kinetic energy of the relative motion is greater than the activation energy of the chemical reaction can collide with chemical reaction.

The collision terms are given by (see Ref. [18] for a detailed derivation)

$$\mathcal{Q}_\alpha^E = \sum_{\beta=1}^4 \mathsf{d}_{\alpha\beta}^2 \int (f_\alpha' f_\beta' - f_\alpha f_\beta) \langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\beta \rangle d\epsilon d\boldsymbol{c}_\beta$$

$$- s\mathsf{d}_{\alpha\gamma}^2 \int (f_\alpha' f_\gamma' - f_\alpha f_\gamma) \qquad (33)$$

$$\times \Theta(\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma \rangle - \Gamma_{\alpha\beta}) \langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma \rangle d\epsilon d\boldsymbol{c}_\gamma$$

$$\mathcal{Q}_\alpha^R = s\mathsf{d}_{\alpha\gamma}^2 \int \left[\left(\frac{\mu_{\alpha\gamma}}{\mu_{\beta\delta}} \right)^3 f_\beta' f_\delta' - f_\alpha f_\gamma \right] \qquad (34)$$

$$\times \Theta(\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma \rangle - \Gamma_{\alpha\beta}) \langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma \rangle d\epsilon d\boldsymbol{c}_\gamma$$

Above, the primes indicate post collisional states, $\mu_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}$ is a reduced mass of the colliding pair,

$\Gamma_{ij} = \sqrt{2\gamma_i/\mu_{ij}}$ is a threshold velocity for the chemical reaction, Θ the Heaviside step function, and s the steric factor. The second term in the right-hand side of Eq. (33) is the correction term that excludes from the total number of collisions those events that lead to chemical reaction when the kinetic energy of the colliding particles is greater than the activation energy.

The SRS model possesses important mathematical properties. At the microscopic level, the model incorporates the correct detailed balance and microscopic reversibility principle, that is direct and reverse collisions of both elastic and reactive types occur with the same probability. At the macroscopic level, the SRS model has good consistency properties (Subsection 2.2) concerning correct chemical exchange rates, conservation laws, entropy production, $\mathcal{H}$-function and trend to equilibrium.

Both microscopic and macroscopic properties asserting the consistency of the SRS model are crucial for the mathematical analysis of the system of partial differential equations of the SRS model. In particular, existence, uniqueness, and stability results can be investigated on the basis of such properties.

6 EXISTENCE RESULT FOR THE SRS MODEL

In this section, the global existence result of Ref. [18], for the extended Boltzmann equations (2), (33) and (34) of the SRS model, is revisited. The proof of the theorem is based on the renormalized theory proposed by DiPerna and Lions in Ref. [19] for the inert one-component Boltzmann equation, and then followed in Ref. [16] for a reactive mixture such that reactive collisions do not cause neither mass transfer nor molecular diameter alteration. The general idea of the proof is here sketched.

We introduce the notation $\mathcal{Q}_\alpha^{E+}$, $\mathcal{Q}_\alpha^{E-}$ to represent the gain and loss terms of the elastic collision operator, and $\mathcal{Q}_\alpha^{R+}$, $\mathcal{Q}_\alpha^{R-}$ with analogous meaning, so that

$$\mathcal{Q}_\alpha^E = \mathcal{Q}_\alpha^{E+} - \mathcal{Q}_\alpha^{E-}, \quad \mathcal{Q}_\alpha^R = \mathcal{Q}_\alpha^{R+} - \mathcal{Q}_\alpha^{R-}$$

6.0.1 DEFINITION.

(Mild solution) Non-negative functions $f_\alpha \in L_{loc}^1(\mathcal{S} \times \mathbb{R}^3; [0, T])$ define a mild solution of the system (2), (33-34) if, for each $T \in]0, \infty[$, the gain and loss terms $\mathcal{Q}_\alpha^{E+}$, $\mathcal{Q}_\alpha^{E-}$, $\mathcal{Q}_\alpha^{R+}$, $\mathcal{Q}_\alpha^{R-}$ are in $L^1(0, T)$,

a.e. in $(\boldsymbol{x}, \boldsymbol{c}_\alpha) \in \mathcal{S} \times \mathbb{R}^3$ and

$$f_\alpha^\#(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) - f_\alpha^\#(\boldsymbol{x}, \boldsymbol{c}_\alpha, s) = \int_s^t \Big[\mathcal{Q}_\alpha^{E\#}(\boldsymbol{x}, \boldsymbol{c}_\alpha, \tau)$$
$$+ \mathcal{Q}_\alpha^{R\#}(\boldsymbol{x}, \boldsymbol{c}_\alpha, \tau) \Big] d\tau, \quad 0 < s < t < T \quad (35)$$

where $f_\alpha^\#(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) = f_\alpha(\boldsymbol{x} + \boldsymbol{c}_\alpha t, \boldsymbol{c}_\alpha, t)$ and similarly for $\mathcal{Q}_\alpha^{E\#}$ and $\mathcal{Q}_\alpha^{R\#}$. $\qquad \square$

6.0.1 THEOREM (GLOBAL EXISTENCE RESULT).
Assume that for $\alpha = 1, \ldots, 4$, the initial distributions $f_{\alpha 0} \geq 0$ are such that

$$\sup_\alpha \iint\limits_{\mathcal{S} \times \mathbb{R}^3} \big(1 + \boldsymbol{x}^2 + \boldsymbol{c}_\alpha^2 + \log^+ f_{\alpha 0}\big) f_{\alpha 0} \, d\boldsymbol{c}_\alpha d\boldsymbol{x} < \infty \quad (36)$$

with $\log^+(z) = \max\{\log(z), 0\}$. Then, there exists a non-negative mild solution $\{f_1, f_2, f_3, f_4\}$ of the system (2), (33-34) with $f_\alpha \in C([0, T]; L^1(\mathbb{R}^3 \times \mathbb{R}^3))$, such that $f_\alpha(t)\big|_{t=0} = f_{\alpha 0}$, for $\alpha = 1, 2, 3, 4$. $\qquad \square$

The result expressed in Theorem 6.0.1 states the existence of a global in time, spatially inhomogeneous, and L^1 solution for the SRS model, provided that the initial mass, momentum, total energy and entropy are finite, as assumed in hypothesis (36).

Sketch of the proof of Theorem 6.0.1. The proof of Theorem 6.0.1 follows similar arguments as in Ref. [16]. It is based on the following tools [19, 16].

(i) A priory estimations of type

$$\sup_\alpha \sup_{t \in [0,T]} \iint\limits_{\mathcal{S} \times \mathbb{R}^3} \big(1 + \boldsymbol{x}^2 + \boldsymbol{c}_\alpha^2 + \log^+ f_\alpha\big) f_\alpha d\boldsymbol{c}_\alpha d\boldsymbol{x} < \infty \quad (37)$$

that are obtained from the conservation laws of total mass, momentum and total energy, as well as from a suitable entropy identity (see Ref. [18]). Bounds (37) assure that there is no infinite concentration of densities in the system governed by Eqs. (2), (33-34).

(ii) Velocity averaging results that, in some sense, transfer the regularity of functions f_α for velocity averaged quantities, such as the macroscopic variables, see Ref. [20]. Velocity averaging results compensate the lack of regularity of the non-linear collision terms.

(iii) Renormalized theory [19], that considers a suitable notion of mild solution, see Definition 6.0.2 below. The method of renormalization introduces a nonlinear change of variable that reformulates the Boltzmann equations (2), (33-34) to an equivalent form, provided that certain bounds are satisfied, see Lemma 6.0.1.

6.0.2 DEFINITION.
(Renormalized solution) Non-negative functions $f_\alpha \in L^1_{loc}(\mathcal{S} \times \mathbb{R}^3; [0, T])$ are renormalized solutions of the system (2), (33-34) if

$$\frac{1}{1 + f_\alpha} \mathcal{Q}_\alpha^{E\pm}, \ \frac{1}{1 + f_\alpha} \mathcal{Q}_\alpha^{R\pm} \in L^1_{loc}(\mathcal{S} \times \mathbb{R}^3; [0, T])$$

$$\frac{\partial}{\partial t} \log(1 + f_\alpha) + \boldsymbol{c}_\alpha \frac{\partial}{\partial \boldsymbol{x}} \log(1 + f_\alpha) = \frac{\mathcal{Q}_\alpha^E + \mathcal{Q}_\alpha^R}{1 + f_\alpha}$$

in the sense of distributions on $[0, T] \times \mathcal{S} \times \mathbb{R}^3$ $\quad \square$

6.0.1 LEMMA.
Non-negative functions $f_\alpha \in L^1_{loc}(\mathcal{S} \times \mathbb{R}^3; [0, T])$ are renormalized solutions of the system (2), (33-34) if and only if they are mild solutions and

$$\frac{1}{1 + f_\alpha} \mathcal{Q}_\alpha^{E\pm}, \ \frac{1}{1 + f_\alpha} \mathcal{Q}_\alpha^{R\pm} \in L^1_{loc}(\mathcal{S} \times \mathbb{R}^3; [0, T])$$

$\qquad \square$

Then the central idea of the proof is to define suitable approximate collision terms $\mathcal{Q}_{\alpha n}^E$ and $\mathcal{Q}_{\alpha n}^R$, with $n = 1, 2, \ldots$, satisfying the main consistency properties of $\mathcal{Q}_\alpha^E$ and $\mathcal{Q}_\alpha^R$, such that the approximate problems

$$\frac{\partial f_\alpha^n}{\partial t} + \sum_{i=1}^3 \boldsymbol{c}_i^\alpha \frac{\partial f_\alpha^n}{\partial \boldsymbol{x}_i} = \mathcal{Q}_{\alpha n}^E + \mathcal{Q}_{\alpha n}^R$$
$$f_\alpha^n(\boldsymbol{x}, \boldsymbol{c}_\alpha, 0) = f_{\alpha 0}^n(\boldsymbol{x}, \boldsymbol{c}_\alpha), \quad \alpha = 1, 2, 3, 4$$

can be studied with known methods for PDE's (semigroup techniques have been used, see [16] for details). Then one takes the weak limit $f_\alpha^n \longrightarrow f_\alpha$ and uses stability results to show that the sequence $\{f_1^n, f_2^n, f_3^n, f_4^n\}$ converges to a renormalized solution of the system (2), (33-34). A crucial part in this passage to the limit is the estimation of the renormalized collision terms, for which the velocity averaging results provide an important tool. $\qquad \square$

6.0.1 REMARK (RELEVANCE OF THEOREM 6.0.1).
The existence result stated in Theorem 6.0.1 has important implications at the level of approximation questions. $\qquad \square$

6.0.2 REMARK (FUTURE PERSPECTIVES).
The spatially homogeneous theory of the SRS model, in which the distribution functions do not depend on the $\boldsymbol{x}$ variable, is a topic of great interest. Some advances have been made in view of studying existence

of solutions, uniqueness and stability results for the homogeneous reactive equations.

Another regime of interest corresponds to the case in which the distribution functions are assumed very close to the equilibrium. In this case, one considers the linearized version of the SRS model around an equilibrium solution and uses the spectral properties of the linearized collision operators to prove existence and stability of close to equilibrium solutions for the SRS system. Some studies have been developed also in this direction. □

REFERENCES

[1] C. Cercignani, "Introduction to Reactive Gas Dynamics", *Oxford University Press*, NewYork, 1998.

[2] S. Chapman and T. G. Cowling, "The Mathematical Theory on Non-Uniform Gases", *Cambridge University Press*, Cambridge, 1999.

[3] V. Giovangigli, "Multicomponent Flow Modeling", *Birkhäuser*, Boston, 1999.

[4] R. Brun, "Introduction to Reactive Gas Dynamics", *Oxford University Press*, NewYork, 2009.

[5] E. Nagnibeda and E. Kustova, "Non-Equilibrium Reacting Gas Flows: Kinetic Theory of Transport and Relaxation Processes", *Springer Verlag*, Berlin, 2009.

[6] G. M. Kremer, "An introduction to the Boltzmann equation and transport processes in gases", *Springer*, Berlin, 2010.

[7] G. M. Kremer, F. S. Oliveira and A. J. Soares, "$\mathcal{H}$- theorem and trend to equilibrium of chemically reacting mixtures of gases", *Kinetic and Related Models* **2** pp. 333-343, 2009.

[8] C. Bardos, F. Golse and D. Levermore, "Fluid Dynamic Limits of Kinetic Equations. I. Formal Derivations", *J. Stat. Phys.*, **63**, pp. 323-344, 1991.

[9] G. M. Kremer and A. J. Soares, "Effect of reaction heat on Maxwellian distribution functions and rate of reactions", *J. Stat. Mech.*, **P12003**, pp. 1-16, 2007.

[10] F. Carvalho and A. J. Soares, "On the dynamics and linear stability of one-dimensional steady detonation waves", *J. Phys. A: Math. Theor.*, **45**, 255501, pp. 1-23, 2012.

[11] W. Fickett, "Introduction to Detonation Theory", *University of California Press*, Berkeley, 1986.

[12] J. H. S. Lee, "The Detonation Phenomenon", *Cambridge University Press*, Cambridge, 2008.

[13] N. Xystris and J. S. Dahler, "Kinetic theory of simple reacting spheres", *J. Chem. Physics*, **68**, pp. 387–401, 1978.

[14] J. S. Dahler and L. Qin, "The kinetic theory of a simple reacting fluid: Scattering functions and relaxation processes", *J. Chem. Physics*, **103**, pp. 725–750, 1995.

[15] J. S. Dahler and L. Qin, "Non-Equilibrium Statistical Mechanics of Chemically Reactive Fluids", *J. Chem. Physics*, **118**, pp. 8396–8404, 2003.

[16] J. Polewczak, "The kinetic theory of simple reacting spheres: I. Global existence results in a dilute-gas limit", *J. Stat. Physics*, **100**, pp. 327–362, 2000.

[17] M. Groppi and J. Polewczak, "On two kinetic models for chemical reactions: comparisons and existence results", *J. Stat. Physics*, **117**, pp. 211–241, 2004.

[18] J. Polewczak and A. J. Soares, "Kinetic theory of simple reacting spheres I", 27th Int. Symp. on Rarefied Gas Dyamics, *AIP Conf. Proc.*, **1333**, pp. 117–122, 2011.

[19] R. L. DiPerna and P. L. Lions, "On the Cauchy problem for the Boltzmann equation: Global existence and weak stability", *Annals of Math*, **30**, pp. 321–366, 1989.

[20] F. Golse, "The Boltzmann Equation and Its Hydrodynamic Limits", in *Evolutionary Equations*, Eds. C. Dafermos, and E. Feireisl, Vol. II, pp. 159–301, Handb. Diff. Equations, *Elsevier*, North-Holland, 2005.