## NUMERICAL CODES FOR MOLECULAR FLUID DYNAMIC PROCESSES WITH INELASTIC INTERACTIONS

C. Cattani<sup>1</sup>, F. Hanser<sup>2</sup>, R. Monaco<sup>3</sup> and M. Pandolfi Bianchi<sup>3</sup>

<sup>1</sup>Dipartimento di Matematica, Università di Roma "La Sapienza", P.le A.Moro, 5 ; I–00185 Roma, Italy; cattani@axrma.uniroma1.it <sup>2</sup>Institut für Theoretische Physik, Technische Universität Graz, Austria; hanser@itp.tu-graz.ac.at <sup>3</sup>Dipartimento di Matematica, Politecnico di Torino, Italy; MONACO@polito.it; MIRIAM@polito.it

## **Extended Abstract**

In the present paper numerical codes, capable to simulate fluid dynamic processes of real gases, are presented as tools useful to quantify phenomenologies characterizing industrial processes at a molecular scale. Moreover, such codes can be implemented on personal computers and can show the real-time evolution of gas systems in some different physical situations. In this work we will refer to processes characterized by elastic and inelastic molecular interactions, namely • gas mixtures undergoing chemical reactions of different type;

• gases with internal energy levels interacting with a radiation field.

In order to obtain the objective specified above it is convenient to construct kinetic models which, at the same time, provide a good and detailed description of this relatively complex phenomenology, are physically selfconsistent, and present a simple mathematical structure. Since these models are derived for a system of particles moving only according to a finite set of selected velocities, their mathematical structure is specially suited to implement the algorithms which will be described further on, in a natural way. The models adopted here are represented by a semilinear set of partial differential equations in the independent variables of time and space. The unknown functions to be computed are the distributions of each gas species and in case of interaction with a radiation field also the distribution of monochromatic photons. On a mathematical ground the fluid dynamic processes are represented by initial boundary value problems in planar geometry, while, on a physical ground, such numerical simulations describe the onset of the processes and their trend to equilibrium.

This paper is divided into three parts:

1) description of the physical system at a molecular level and features of the related family of mathematical models;

2) formulation of initial-boundary value problems and discussion of the related algorithms implemented in the numerical codes;

3) use of the codes, description and visualization of the outputs.

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**Mathematical Modeling** <u>Models for reactive flows</u>. In the present paper, reacting gases with autocatalytic and bimolecular reactions are considered. In the former, diatomic molecules  $A_2$  in presence of atoms A and  $A^*$  with different energy levels undergo both elastic collisions and inelastic interactions according to the reversible chemical reaction  $A_2 + M \rightleftharpoons A + A^* + M$  where the catalyst M can be  $A, A^*$ , or  $A_2$ . In the latter, four gas species A, B, C, D interact according to the following reversible reaction  $A + B \rightleftharpoons C + D$ . Such reactive flows are modeled by the following kinetic equations [1,2]

$$\frac{\partial N_i^r}{\partial t} + \vec{v}_i^r \cdot \vec{\nabla} N_i^r = J_i^r(\underline{N}) + \mathcal{R}_i^r(\underline{N}) = Q_i^r(\underline{N}) . \tag{1}$$

In Eq.(1),  $N_i^r$  (components of the vector  $\underline{N}$ ) are the distribution functions of particles A,  $A^*$ , and  $A_2$ , or A, B, C, D, with velocities  $\vec{v}_i^r$ , i being the index joined to the selected velocity directions, and  $J_i^r$  and  $\mathcal{R}_i^r$  are the corresponding nonlinear terms due to elastic collisions and collisions with chemical reactions, respectively.

<u>Models for gases in presence of a photon field</u>. Consider a gas of atoms  $A_1$  and  $A_2$ , with only two internal energy levels  $E_1$  and  $E_2$ , interacting with a radiation field of photons p at a fixed frequency  $\nu = (E_2 - E_1)/h$ , h being the Planck constant. Besides elastic and inelastic collisions among gas particles, the interaction between atoms and photons occurs in one of the following way:

$$A_1 + p \rightarrow A_2, \qquad A_2 \rightarrow A_1 + p, \qquad A_2 + p \rightarrow A_1 + 2p.$$

The kinetic equations [3] of the above system are

$$\frac{\partial f_i^r}{\partial t} + \vec{v}_i^r \cdot \vec{\nabla} f_i^r = J_i^r(\underline{f}) + \mathcal{R}_i^r(\underline{f}) + \mathcal{P}_i^r(\underline{f}, I) = Q_i^r(\underline{f}, I)$$
(2)

$$\frac{\partial I}{\partial t} + c\vec{\Omega} \cdot \vec{\nabla}I = ch\nu [n_2(\alpha + \beta I) - n_1\beta I].$$
(3)

In Eqs.(2,3),  $f_i^r$ ,  $n_r$ , r = 1, 2 are the distributions and number densities of the gas particles  $A_1$  and  $A_2$ .  $J_i^r$  and  $\mathcal{R}_i^r$  are the terms due to elastic and inelastic collisions, whereas  $\mathcal{P}_i^r$  refer to interaction between atoms and photons. In Eq.(3)  $I = I(t, \mathbf{x}, \Omega)$  denotes the radiation intensity,  $c\vec{\Omega}$  being the light velocity, and  $\alpha$ ,  $\beta$  are the Einstein coefficients of photon absorption and emission.

**Thermodynamical equilibrium** In order to validate the above models from a physical point of view it is necessary to determine the equilibrium solutions to Eqs. (1-3) which provide the mechanical and chemical equilibrium state for Eq.(1) and the thermodynamical equilibrium state between the atom populations  $n_1$ ,  $n_2$ , and the radiation field for Eqs.(2-3). These derivations will be then used in the process simulations to show their trend to equilibrium. For what concerns Eq.(1) the equilibrium is provided by putting separately  $J_i^r(\underline{N})$ 

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and  $\mathcal{R}_{i}^{r}(\underline{N})$  equal to zero.  $J_{i}^{r} = 0$  permits to express explicitly the Maxwellian distributions, while  $\mathcal{R}_{i}^{r} = 0$  exhibits the mass action law which rules chemical equilibrium. Analogously, Maxwellian distributions and a law governing equilibrium between the two populations  $n_{1}$ ,  $n_{2}$  are obtained, as well, by setting  $J_{i}^{r}(\underline{N}) = \mathcal{R}_{i}^{r}(\underline{N}) = 0$  in Eq.(2). The simultaneous vanishing of  $\mathcal{P}_{i}^{r}(\underline{f}, I)$  and right-hand-side of Eq.(3) allows to recover the so-called Planck's radiation law which rules equilibrium of the gas particles in presence of a radiation field. This law consists in an explicit functional relation between the equilibrium intensity of the field and gas temperature.

Simulations and use of the numerical codes The simulations proposed consist in the integration, with respect to time and space, of Eqs.(1-3) in a slab. In mathematical terms, this means that we have to solve Eq.(1) or Eqs.(2-3) joined to suitable initial and boundary conditions.

For the models of reacting gases (for both bimolecular and autocatalytic reactions), as initial data, we consider gases in different thermodynamical equilibrium states. For what concerns boundary conditions, the gas particles are reflected by the boundaries of the slab according to a specular reflection law. The simulations provide then the description of the onset of chemical reactions and the evolution of the system from chemical disequilibrium to equilibrium.

For the model of gases with internal energy levels and monochromatic photons we show simulations of the following problem, referred to, in literature, as the Milne–Chandrasekhar problem: at time t = 0, thermodynamical equilibrium (including Planck's law) and specular reflection on the slab boundaries for both atoms and photons; at time  $t = 0^+$ , specular reflection for atoms only, constant illumination on the right boundary and total absorption of photons on the left one. The simulation shows the transient behaviour of the system and its relaxation to a new thermodynamical equilibrium state.

**Numerical method** The numerical method adopted for such simulations is the known "Fractional Step Method", here specifically developed for kinetic equations including dissipative interaction terms. In particular, after each time step of integration, the distribution functions are corrected in order to assure conservation of mass, momentum and total (kinetic and internal) energy, according the procedure proposed in [4].

## References

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