Numerical approximation of a BGK-type relaxation model for reactive mixtures

A. Aimi, M. Diligenti, M. Groppi, C. Guardasoni

Department of Mathematics, University of Parma
V.le G.P. Usberti, 53/A, 43100 Parma, Italy

`alessandra.aimi,mauro.diligenti,maria.groppi@unipr.it`

1 Introduction

The mathematical modelling for practical purposes of multi-component gaseous flows with chemical reactions is an important research fields, and in this context several kinetic approaches have been developed in the last decades, starting from the pioneering work by Prigogine-Xhrouet ([7]). The increasing interest on kinetic models is mainly motivated by the fact that they enable the macroscopic laws to be derived from elementary principles, providing consistent macroscopic theories in the hydrodynamic limit, and moreover they allow to deduce transport and structure coefficients, that are not directly obtainable from macroscopic approaches. The so called BGK equations ([3]) constitute a well known model of the nonlinear Boltzmann equation and a simpler tool of investigation in particular for reacting gaseous flows, for which the collisional part of the relevant kinetic equations becomes much heavier. A recent consistent BGK-type approach for inert gas mixtures and its extension to reacting gas mixtures, according to a Boltzmann-like kinetic model has been developed in [8] for a bimolecular reversible chemical reaction. These models are based on the simple idea of introducing only one BGK collision operator for each species s, taking into account all interactions with whatever species r.

In this communication we propose a numerical strategy to simulate the reactive BGK equations in more general space-dependent conditions. In particular we focus here on problems with axial symmetry, which are of interest in many applications like for instance the classical evaporation-condensation problem. The method is based on time splitting techniques, which are widely used in the numerical analysis of the classical Boltzmann equation ([4]), but their application to kinetic systems describing reacting gas mixtures has not already been discussed, to our knowledge. The time splitting approach has the advantage of simplifying the problem by treating separately the two steps, the convection or transport step, which solves the free-streaming equations, and the collision step, which solves the spatially homogeneous BGK equations. The numerical solution of this latter step, which can be regarded as a Cauchy problem, is evaluated with explicit Runge-Kutta (RK) schemes of different order. Numerical results on time-dependent Riemann problem for mixture of 4 gases are presented.

2 Model equations and numerical approximation

The BGK approximation introduced in [6] for the chemical reaction model of Boltzmann-type is described by the following kinetic equations

$$(2.1) \qquad \frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \frac{\partial f^s}{\partial \mathbf{x}} = \nu_s \big(\mathcal{M}_s - f^s \big), \qquad s = 1, \dots, 4,$$

where f^s are distribution functions and $\mathcal{M}_s$ is an auxiliary local Maxwellian depending on velocity vector variable $\mathbf{v}$, masses m^s and disposable parameters $n_s, \mathbf{u}_s, T_s$:

$$(2.2) \qquad \mathcal{M}_s = n_s \left(\frac{m^s}{2\pi K T_s} \right)^{\frac{3}{2}} \exp\left[-\frac{m^s}{2K T_s}(\mathbf{v} - \mathbf{u}_s)^2 \right], \qquad s = 1, \ldots, 4.$$

At last in (2.1), ν_s represents the inverse of the s-th relaxation time, possibly depending on macroscopic fields, but independent of $\mathbf{v}$. The above auxiliary fields n_s, $\mathbf{u}_s$, T_s are determined from the corresponding actual moments of the distribution functions f^s (namely number density n^s, mass velocity $\mathbf{u}^s$ and temperature T^s of each component) by requiring that the exchange rates for mass, momentum and total (kinetic plus chemical) energy prescribed by (2.1) coincide with those deduced from the reactive Boltzmann equations (see [6] for a detailed derivation). We consider here the application of BGK equations (2.1) to problems with axial symmetry with respect to an axis (say, $x_1 \equiv x$), in the sense that all transverse spatial gradients vanish, and the gas is drifting only in the axial direction. In such cases, distribution functions f^s depend on the full velocity vector $\mathbf{v}$, but dependence on the azimuthal direction around the symmetry axis is such that all transverse components of the macroscopic velocities $\mathbf{u}^s$ vanish (i.e. $u_2^s = u_3^s = 0$). Let us introduce the new unknowns

$$(2.3) \qquad \phi_1^s(x, v, t) = \int_{\mathbb{R}^2} f^s \, \mathrm{d}v_2 \mathrm{d}v_3, \qquad \phi_2^s(x, v, t) = \int_{\mathbb{R}^2} (v_2^2 + v_3^2) f^s \, \mathrm{d}v_2 \mathrm{d}v_3,$$

each depending only on one space and one velocity variable. From the system (2.1) we can obtain the following system of BGK equations for the unknown vector $\underline{\phi}^s = (\phi_1^s, \phi_2^s)^\top$ (Chu's reduction [5]), coupled with initial conditions

$$(2.4) \qquad \begin{cases} \dfrac{\partial \underline{\phi}^s}{\partial t} + v \dfrac{\partial \underline{\phi}^s}{\partial x} = \nu_s(\underline{\phi}_s^e - \underline{\phi}^s) & t > 0, \ x \in \mathbb{R}, \ v \in \mathbb{R}, \qquad s = 1, \ldots, 4 \\[2ex] \underline{\phi}^s(x, v, 0) = \underline{\phi}_0^s(x, v) \end{cases}.$$

The BGK equations (2.4) drift the relaxation process towards the vector functions $\underline{\phi}_s^e = \left(\phi_{s,1}^e, \phi_{s,2}^e \right)^\top$, which is obtained by Chu's transform of (2.2) and has the form

$$(2.5) \qquad \left(\phi_{s,1}^e, \phi_{s,2}^e \right)^\top = \left(M_s, \frac{2K T_s}{m^s} M_s \right)^\top, \quad M_s = n_s \left(\frac{m^s}{2\pi K T_s} \right)^{1/2} \exp\left[-\frac{m^s}{2K T_s}(v - u_s)^2 \right].$$

This transformation reduces the auxiliary velocity to a scalar parameter u_s, owing to the axial symmetry. To determine n_s, u_s, T_s it is necessary first to compute the exchange rates for the Boltzmann reactive model described in [6] and [8]. Such rates are known analytically for Maxwell molecules, even in the chemical frame by assuming moderately slow chemical reactions (for a detailed derivation see [6]). Those rates involve fundamental macroscopic moments of distribution functions f^s, which are given in terms of ϕ_1^s and ϕ_2^s. We point out that the unknowns ϕ_1^s and ϕ_2^s provide a reduced description of the velocity distributions, if compared to f^s, but they suffice for our purposes. The macroscopic collision frequencies ν_s, which measure the strength at which BGK model equations push distributions towards equilibrium, can be evaluated by a suitable estimation of the actual average number of collisions taking place for each species (see [6]). It is remarkable that

the consistency properties of the reactive BGK model, proved in [6], are independent from the choice of macroscopic collision frequencies.

We rewrite here the system (2.4) pointing out, in particular, the dependence of the vector functions $\underline{\phi}^e_s$ and of the macroscopic collision frequencies ν_s on the components of the unknown vector solution $\underline{\Phi} = (\underline{\phi}^1, \underline{\phi}^2, \underline{\phi}^3, \underline{\phi}^4)^\top$. Hence, we consider the following equivalent one-dimensional initial-value hyperbolic nonlinear problem

$$(2.6) \quad \begin{cases} \dfrac{\partial \underline{\phi}^s}{\partial t} + v \dfrac{\partial \underline{\phi}^s}{\partial x} = \nu_s(\underline{\Phi}) \left[\underline{\phi}^e_s(\underline{\Phi}) - \underline{\phi}^s \right], \quad s = 1, \cdots, 4; \quad t > 0, \, x \in \mathbb{R}, \, v \in \mathbb{R}, \\[2mm] \underline{\phi}^s(x, v, 0) = \underline{\phi}^s_0(x, v), \end{cases}$$

for the unknowns $\underline{\phi}^s = (\phi^s_1, \phi^s_2)^\top$, $s = 1, \cdots, 4$. Problem (2.6) can be rewritten in the form

$$(2.7) \quad \begin{cases} \dfrac{\partial \underline{\phi}^s}{\partial t} = A[\underline{\phi}^s] + B[\underline{\phi}^s], \quad s = 1, \ldots, 4; \quad t > 0, \, x \in \mathbb{R}, \, v \in \mathbb{R}, \\[2mm] \underline{\phi}^s(x, v, 0) = \underline{\phi}^s_0(x, v), \end{cases}$$

where

$$A[\underline{\phi}^s] = -v \frac{\partial \underline{\phi}^s}{\partial x}, \text{ convection operator; } \quad B[\underline{\phi}^s] = \nu_s(\underline{\Phi}) \left[\underline{\phi}^e_s(\underline{\Phi}) - \underline{\phi}^s \right], \text{ collision operator.}$$

Therefore, in order to compute numerically the solution, it is usual to solve

$$\frac{\partial \underline{\phi}^s}{\partial t} = A[\underline{\phi}^s] \qquad \text{and} \qquad \frac{\partial \underline{\phi}^s}{\partial t} = B[\underline{\phi}^s]$$

separately. This procedure is known as a splitting method and it is widely used in the numerical analysis of the Boltzmann equation. The method consists of two steps, the convection step, which solves the collision-less equation (free-transport equation), and the collision step, which solves the space-homogeneous equation. Setting the solution $\underline{\Phi}(t)$ of the problem (2.7) as $\underline{\Phi}(t) = S^t_{A+B}(\underline{\Phi}_0)$, where: $\underline{\Phi}_0 = (\underline{\phi}^1_0, \underline{\phi}^2_0, \underline{\phi}^3_0, \underline{\phi}^4_0)^\top$, the conventional splitting method (CSM) is nothing more than (see [4]):

$$(2.8) \qquad\qquad S^{\Delta t}_{A+B} = S^{\Delta t}_A S^{\Delta t}_B + O(\Delta t^2).$$

The accuracy per time step may be improved by Strang's splitting method (SSM):

$$(2.9) \qquad\qquad S^{\Delta t}_{A+B} = S^{\Delta t/2}_A S^{\Delta t}_B S^{\Delta t/2}_A + O(\Delta t^3).$$

For the numerical implementation of splitting techniques, at first, we have to define a finite numerical domain in the phase space: $[x_L, x_R] \times [v_L, v_R]$ dependent on the problem data: in particular the choice of $[v_L, v_R]$ is related to the initial velocity distribution while the choice of $[x_L, x_R]$ depends on the observation time interval. Consequently, we impose the following conditions (at infinity) for all v and t

$$\underline{\phi}^s(x, v, t) = \underline{\phi}^s(x_L, v, t) \quad x \leq x_L, \qquad \underline{\phi}^s(x, v, t) = \underline{\phi}^s(x_r, v, t) \quad x \geq x_R.$$

Let $x_r = x_L + r\Delta x$, $r = 0, \cdots, N_x$ and $v_q = v_L + q\Delta v$, $q = 0, \cdots, N_v$, be uniform grids defined in $[x_L, x_R]$ and in $[v_L, v_R]$, respectively. Having set $\underline{\psi}^s(x_r, v_q, 0) = \underline{\phi}^s_0(x_r, v_q)$ and

$t_i = i\,\Delta t$, $i = 0, \cdots, N-1$, in the convection step, the problem is to evaluate the formal solution at time t_{i+1}, because it should be obtained from the initial condition evaluated at time t_i along the characteristic lines, but $\underline{\psi}^s$ is known only in the original nodes of the grid. To overcome this difficulty, we have considered the following algorithm:

$*$ compute the nearest grid point from $x_r - v_q\Delta t$, named x_j;

$*$ compute $\underline{\psi}^s(x_r - v_q\Delta t, v_q, t_i)$ using Taylor expansion around x_j truncated at a suitable order p, with derivatives approximated with centered finite differences at the same accuracy (see [2]).

Note that for $k = 2, 3$, the order p is chosen such that: $(\Delta x)^{p+1} \leq (\Delta t)^k$, to preserve the accuracy order per time step of the chosen splitting procedure. In order to avoid numerical instability near spatial edges $x = x_L$, $x = x_R$, the extrapolation, which causes the instability, is never used. Furthermore, for the same reason, it is useful to choose the space and time steps satisfying the following Courant-Friedrichs-Lewy (CFL) condition: $\Delta x/2 \geq \Delta t \max\{|v_L|, |v_R|\}$. For the numerical solution of collision steps, we compute a numerical approximation of the moments of $\underline{\psi}^s$ needed in $\underline{\phi}_s^e(\underline{\Psi})$ using composite Simpson rule over $[v_L, v_R]$. The velocity step Δv is chosen to assure the double precision accuracy to the numerical approximation of the moments related to the initial data. Then, time-advancing is carried out using explicit RK methods of order k-1, k=2, 3, which maintain the overall accuracy of CSM and SSM, respectively.

References

1. P. Andries, K. Aoki and B. Perthame, A consistent BGK-type model for gas mixtures, *J. Stat. Phys.*, vol. 106, 2002, 993–1018.
2. W.G. Bickley, Formulae for Numerical Differentiation, *Math. Gazette*, vol. 25, 1941, 19.
3. P.L. Bhatnagar, E.P. Gross and K. Krook, A model for collision processes in gases, *Phys. Rev.*, vol. 94, 1954, 511–524.
4. A.V. Bobylev and T. Ohwada, On the generalization of Strang's splitting scheme, *Riv. Mat. Univ. Parma*, vol. 6(2*), 1999, 235–243.
5. C.K. Chu, Kinetic-theoretic description of the formation of a shock wave, *Phys. Fluids*, vol. 8, 1965, 12–22.
6. M. Groppi and G. Spiga, A Bhatnagar–Gross–Krook–type approach for chemically reacting gas mixtures, *Physics of Fluids*, vol. 16, 2004, 4273–4284.
7. I. Prigogine and E. Xhrouet, On the perturbation of Maxwell distribution function by chemical reaction in gases, *Physica*, vol. XV, 1949, 913–932.
8. A. Rossani and G. Spiga, A note on the kinetic theory of chemically reacting gases, *Physica A*, vol. 272, 1999, 563–573.