

NUMERICAL APPROXIMATION OF A BGK-TYPE RELAXATION MODEL FOR REACTIVE MIXTURES

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A consistent BGK-type approach to reacting gas mixtures, according to Boltzmann-like kinetics for a bimolecular reversible chemical reaction has been recently introduced. In this paper we apply a numerical strategy based on time splitting techniques to simulate the reactive BGK equations. These techniques have the advantage of simplifying the problem by treating separately the convection step and collision step. Numerical results of the time-dependent Riemann problem for the reactive BGK system are presented.

Keywords: Boltzmann equation, BGK model, reacting mixtures, Riemann problem, splitting methods

1. Introduction

In recent years, new suggestions and proposals concerning the mathematical modelling and applications of multi-component gaseous flows with chemical reactions have been published. In this context, several kinetic approaches have been developed in the last decades, starting from the pioneering work by Prigogine-Xhrouet.¹ 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 interested reader is referred to the comprehensive Ref. 2). The so called BGK equations^{3,4} constitute a well known model of the non-linear Boltzmann equation and a simpler tool of investigation in particular for reacting gaseous flows, for which the collision part of the kinetic equations becomes much heavier. A recent extension of a consistent BGK-type approach for inert gas mixtures to reacting gases, according to a Boltzmann-

like kinetic model developed in Ref. 5 for a bimolecular reversible chemical reaction of the type: $A^1 + A^2 \rightleftharpoons A^3 + A^4$, has been investigated in Ref. 6. This model is based on the simple idea of introducing only one suitable BGK collision operator for each species s , taking into account all interactions with whatever species r .

Here we propose a numerical strategy to simulate the reactive BGK equations in more general space-dependent situations. 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.⁷ The method is based on time splitting techniques, which are widely used in the numerical analysis of the classical Boltzmann equation⁸⁻¹⁰ but their application to kinetic systems describing reacting gas mixtures has not been yet 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 along the characteristic lines, and the collision step, which solves the spatially homogeneous BGK equations. The numerical solution of this latter, which can be regarded as a Cauchy problem, is evaluated with Runge-Kutta explicit schemes of different order. Here we consider a splitting method, for which the truncation error per time step Δt is $O(\Delta t^3)$, but due to the accumulation of errors, the convergence rate is $O(\Delta t^2)$ coupled with an explicit Runge-Kutta method of order 2. Numerical results on time-dependent Riemann problem for reacting mixtures of four gases are presented.

2. Model equations

The BGK approximation introduced in Ref. 6 of the Boltzmann-type model worked out in Ref. 5 for chemical reactions is described by the following kinetic equations

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

where f^s is the general distribution function, \mathcal{M}_s is an auxiliary local Maxwellian depending on velocity vector variable \mathbf{v} , molecular masses m^s , Boltzmann constant K and disposable parameters n_s, \mathbf{u}_s, T_s :

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

At last in (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 (1) coincide with those deduced from the reactive Boltzmann equations (see Ref. 5, 6 for a detailed derivation). In presence of chemical reactions, these exchange rates can be made explicit under the assumption of dominant elastic collisions and thus of “slow” chemical reactions (the so called tempered reaction regime), as for instance in the carbon-oxygen chain. We consider the application of BGK equations (1) to problems with axial symmetry with respect to an axis (say, $x_1 \equiv x$). In such cases, the distribution functions f^s depend on \mathbf{v} only through its modulus and its latitudinal angle with respect to that axis, and all transverse components of the macroscopic velocities \mathbf{u}^s vanish (i.e. $u_2^s = u_3^s = 0$). As well known in the literature,¹¹ in this case a reduction to a fully one-dimensional problem is possible, though describing still a three-dimensional velocity space, with a sensible simplification of the computational apparatus. This kind of problem is not only important for theoretical investigation, but also quite frequent in practical applications.⁷

Let us introduce the new unknowns

$$\phi_1^s(x, v, t) = \int_{\mathbb{R}^2} f^s dv_2 dv_3, \quad \phi_2^s(x, v, t) = \int_{\mathbb{R}^2} (v_2^2 + v_3^2) f^s dv_2 dv_3, \quad (3)$$

each depending only on one space and one velocity variable. Starting from (1) and using Chu reduction¹¹ we obtain the following system of BGK equations for the unknown vector $\underline{\phi}^s = (\phi_1^s, \phi_2^s)^\top$, coupled with initial conditions

$$\begin{cases} \frac{\partial \underline{\phi}^s}{\partial t} + v \frac{\partial \underline{\phi}^s}{\partial x} = \nu_s (\underline{\phi}_s^e - \underline{\phi}^s) & t > 0, \quad x \in \mathbb{R}, \quad v \in \mathbb{R}, \quad s = 1, \dots, 4; \\ \underline{\phi}^s(x, v, 0) = \underline{\phi}_0^s(x, v). \end{cases} \quad (4)$$

The BGK equations (4) describe a relaxation process towards the vector functions $\underline{\phi}_s^e = (\phi_{s,1}^e, \phi_{s,2}^e)^\top$, which is obtained by Chu transform of (2) and has the form

$$\begin{aligned} (\phi_{s,1}^e, \phi_{s,2}^e)^\top &= \left(M_s, \frac{2KT_s}{m^s} M_s \right)^\top, \\ M_s &= n_s \left(\frac{m^s}{2\pi KT_s} \right)^{1/2} \exp \left[-\frac{m^s}{2KT_s} (v - u_s)^2 \right]. \end{aligned} \quad (5)$$

The Chu transform reduces the auxiliary velocity to a scalar parameter u_s , owing to the axial symmetry. To determine the auxiliary parameters $n_s = n_s(x, t)$, $u_s = u_s(x, t)$, $T_s = T_s(x, t)$ it is necessary first to compute

the exchange rates for the Boltzmann reactive model described in Ref. 5; such rates are known analytically for Maxwell molecules,¹² even in the tempered reaction regime, and besides may be expressed in terms of mass m^s of each component of the mixture (with $m^1+m^2=m^3+m^4=M$), energies of chemical link E^s , and energy difference between reactants and products $\Delta E = -\sum_{s=1}^4 \lambda^s E^s$ (with $\lambda^1 = \lambda^2 = -\lambda^3 = -\lambda^4 = 1$), conventionally assumed to be positive. Those rates (not reported here for brevity) involve fundamental macroscopic moments of distribution functions f^s , which are given in terms of ϕ_1^s and ϕ_2^s as

$$n^s = \int_{\mathbb{R}} \phi_1^s dv, \quad u^s = \frac{1}{n^s} \int_{\mathbb{R}} v \phi_1^s dv, \quad T^s = \frac{m^s}{3Kn^s} \int_{\mathbb{R}} [(v-u^s)^2 \phi_1^s + \phi_2^s] dv. \quad (6)$$

Here u^s denotes the first component of the mass velocity, since axial symmetry implies $u_2^s = u_3^s = 0$ (and for the same reason $u_{s,2} = u_{s,3} = 0$). 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. In (5), the auxiliary parameters: n_s , u_s , T_s are determined by requiring that the BGK scheme prescribes the same exchange rates of the Boltzmann model. The resulting expressions, as well as a clear derivation and a complete description may be found in Ref. 6. The discussion involves also the global macroscopic parameters: number density n , mass density ρ , mass velocity u , scalar pressure p or temperature T , which are expressed in terms of single component parameters by

$$\begin{aligned} n &= \sum_{s=1}^4 n^s, & \rho &= \sum_{s=1}^4 \rho^s = \sum_{s=1}^4 m^s n^s, & u &= \frac{1}{\rho} \sum_{s=1}^4 m^s n^s u^s, \\ p &= nKT = \sum_{s=1}^4 n^s KT^s + \frac{1}{3} \sum_{s=1}^4 m^s n^s (u^s - u)^2. \end{aligned} \quad (7)$$

The macroscopic collision frequencies $\nu_s = \nu_s(x, t)$, 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.⁶ It is remarkable that the consistency properties of the reactive BGK model, proved in Ref. 6, are independent from the choice of macroscopic collision frequencies. Anyway, a suitable evaluation is needed in order to avoid artificial acceleration or slowing down of the relaxation process.

3. Numerical approximation

We rewrite here the system (4) pointing out, in particular, the dependence of the vector functions $\underline{\phi}_s^e$ and of the macroscopic collision frequencies ν_s on the components of the unknown vector solution $\underline{\Phi} = (\phi^1, \phi^2, \phi^3, \phi^4)^\top$. In fact the auxiliary parameters n_s, u_s, T_s , appearing in (5), as well as the frequencies ν_s , follow from the definition of macroscopic moments of the solution through (7). Hence, we consider the following equivalent one-dimensional (in both space and velocity) initial-value nonlinear problem

$$\begin{cases} \frac{\partial \underline{\phi}^s}{\partial t} + v \frac{\partial \underline{\phi}^s}{\partial x} = \nu_s(\underline{\Phi}) \left[\underline{\phi}_s^e(\underline{\Phi}) - \underline{\phi}^s \right], & s = 1, \dots, 4; \quad t > 0, x \in \mathbb{R}, v \in \mathbb{R}, \\ \underline{\phi}^s(x, v, 0) = \underline{\phi}_0^s(x, v), \end{cases} \quad (8)$$

for the unknowns $\underline{\phi}^s = (\phi_1^s, \phi_2^s)^\top$. Problem (8) can be rewritten in the form

$$\begin{cases} \frac{\partial \underline{\phi}^s}{\partial t} = A[\underline{\phi}^s] + B[\underline{\phi}^s], & s = 1, \dots, 4; \quad t > 0, x \in \mathbb{R}, v \in \mathbb{R}, \\ \underline{\phi}^s(x, v, 0) = \underline{\phi}_0^s(x, v), \end{cases} \quad (9)$$

where: $A[\underline{\phi}^s] = -v \frac{\partial \underline{\phi}^s}{\partial x}$ is the convection operator, and $B[\underline{\phi}^s] = \nu_s(\underline{\Phi}) \left[\underline{\phi}_s^e(\underline{\Phi}) - \underline{\phi}^s \right]$ is the collision operator. Therefore, in order to compute numerically the solution, it is usual to solve: $\frac{\partial \underline{\phi}^s}{\partial t} = A[\underline{\phi}^s]$ and $\frac{\partial \underline{\phi}^s}{\partial t} = B[\underline{\phi}^s]$, separately. This procedure is known as a splitting method and it is a common tool for the numerical analysis of the Boltzmann equation. The method consists of two steps, the convection step, which solves the collisionless equation (free-transport equation), and the collision step, which solves the space-homogeneous equation. Setting the solution $\underline{\Phi}(t)$ of the problem (9) as $\underline{\Phi}(t) = S_{A+B}^t(\underline{\Phi}_0)$, where: $\underline{\Phi}_0 = (\phi_0^1, \phi_0^2, \phi_0^3, \phi_0^4)^\top$, the conventional splitting method (CSM) is nothing more than the following approximation of the operator $S_{A+B}^{\Delta t}$

$$S_{A+B}^{\Delta t} \approx S_B^{\Delta t} S_A^{\Delta t}, \quad (10)$$

for which it holds⁸

$$S_{A+B}^{\Delta t}(\underline{\Phi}_0) = S_B^{\Delta t}[S_A^{\Delta t}(\underline{\Phi}_0)] + \frac{\Delta t^2}{2} [A'_{\underline{\Phi}_0} B(\underline{\Phi}_0) - B'_{\underline{\Phi}_0} A(\underline{\Phi}_0)] + O(\Delta t^3). \quad (11)$$

In spite of this result, because of the accumulation of errors, the convergence rate over $[0, N\Delta t]$ is $O(\Delta t)$. Note that the order of accuracy of this simple splitting does not improve even if we solve analytically both collision and

convection steps. In the CSM, the collision step may also be performed before the convection step, having

$$S_{A+B}^{\Delta t}(\Phi_0) = S_A^{\Delta t}[S_B^{\Delta t}(\Phi_0)] - \frac{\Delta t^2}{2}[A'_{\Phi_0}B(\Phi_0) - B'_{\Phi_0}A(\Phi_0)] + O(\Delta t^3). \quad (12)$$

In this case, the leading term of the truncation error differs only in sign from that one obtained by (11) (see Ref. 8). From this last remark, we deduce a $O(\Delta t^3)$ accuracy per time step for the following approximation of the operator $S_{A+B}^{\Delta t}$

$$S_{A+B}^{\Delta t} \approx \frac{S_A^{\Delta t}S_B^{\Delta t} + S_B^{\Delta t}S_A^{\Delta t}}{2}, \quad (13)$$

i.e., the mean of two applications of CSM with inverted steps: convection-collision and collision-convection. In this way the leading errors of the above methods cancel each other. Moreover, the convergence rate over $[0, N\Delta t]$, due to the accumulation of errors, is $O(\Delta t^2)$, Ref. 8. Other higher order splittings can be found in Ref. 10.

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 distributions while the choice of $[x_L, x_R]$ depends on the observation time interval. Consequently, we impose the following conditions (at infinity) for $s = 1, \dots, 4$,

$$\begin{aligned} \underline{\phi}^s(x, v, t) &= \underline{\phi}^s(x_L, v, t) & x \leq x_L, \quad \forall v, \forall t \\ \underline{\phi}^s(x, v, t) &= \underline{\phi}^s(x_R, v, t) & x \geq x_R, \quad \forall v, \forall t. \end{aligned}$$

Let $x_r = x_L + r\Delta x$, $r = 0, \dots, N_x$ and $v_q = v_L + q\Delta v$, $q = 0, \dots, N_v$, be uniform grids defined in $[x_L, x_R]$ and in $[v_L, v_R]$, respectively.

Having set $\underline{\psi}^s(x_r, v_q, 0) = \underline{\phi}_0^s(x_r, v_q)$ and $t_i = i\Delta t$, for $i = 0, \dots, N-1$, the realization of conventional splitting method (10) is as follows

Convection step:

$$\begin{cases} \frac{\partial \underline{\varphi}^s}{\partial t} + v \frac{\partial \underline{\varphi}^s}{\partial x} = 0, & t_i < t \leq t_{i+1} \\ \underline{\varphi}^s(x_r, v_q, t_i) = \underline{\psi}^s(x_r, v_q, t_i) \end{cases}$$

with formal solution: $\underline{\varphi}^s(x_r, v_q, t_{i+1}) = \underline{\psi}^s(x_r - v_q\Delta t, v_q, t_i)$ and

Collision step:

$$\begin{cases} \frac{\partial \underline{\psi}^s}{\partial t} = \nu_s(\underline{\Psi}) [\underline{\phi}_s^e(\underline{\Psi}) - \underline{\psi}^s], & t_i < t \leq t_{i+1} \\ \underline{\psi}^s(x_r, v_q, t_i) = \underline{\varphi}^s(x_r, v_q, t_{i+1}) \end{cases}$$

where $\underline{\Psi} = (\underline{\psi}^1, \underline{\psi}^2, \underline{\psi}^3, \underline{\psi}^4)^\top$.

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.¹³

To preserve the accuracy order per time step of the chosen splitting procedure, namely $k = 2, k = 3$ for CSM and (13), respectively, the order p is chosen such that: $(\Delta x)^{p+1} \leq (\Delta t)^k$. For this accuracy purpose, we have evaluated $\underline{\psi}^s(x_r - v_q \Delta t, v_q, t_i)$ with Taylor expansion rather than linear interpolation. Furthermore, for the same reason, it is useful to choose the space and time steps satisfying the following Courant-Friedrichs-Lewy (CFL) condition

$$\frac{\Delta x}{2} > \Delta t \max\{|v_L|, |v_R|\}. \quad (14)$$

Note that from (14) we have $\frac{\Delta x}{2} > \Delta t |v_q|$, with $\min\{|v_L|, |v_R|\} \leq |v_q| \leq \max\{|v_L|, |v_R|\}$ and in the foregoing algorithm, the nearest grid point from $x_r - v_q \Delta t$ is always x_r .

In the discretization process the time step Δt and the space step Δx are proportional to one another, i.e., $\Delta t = \lambda \Delta x$ for some positive constant λ . For the numerical solution of collision steps, we compute a numerical approximation of the moments of $\underline{\psi}^s$ needed in $\underline{\phi}_g^e(\underline{\Psi})$ using composite Simpson rule over $[v_L, v_R]$. The velocity step Δv is chosen to assure the double precision stability to the numerical approximation of the moments related to the initial data. Then, time-advancing is carried out using classical explicit Runge-Kutta methods of order $k - 1$, $k = 2, 3$. This choice maintains the overall accuracy order of CSM and of the method (13), respectively.

4. The Riemann problem for reacting mixtures of 4 gases

In this section we present some results related to one-dimensional time-dependent Riemann problem for reactive gaseous flows. This problem starts

from piecewise-constant initial data, having a single discontinuity

$$\underline{\phi}_0^s(x, v) = \begin{cases} \underline{\phi}_{0L}^s(x, v) & x \leq x^* \\ \underline{\phi}_{0R}^s(x, v) & x > x^* \end{cases} \quad (15)$$

We consider elastic microscopic collision frequencies ν_k^{rs} , $k = 0, 1$, defined in Ref. 6, constant with respect to the impact speed and affected by a factor $1/\varepsilon = 10^l$, where ε is the Knudsen number, which corresponds to approach the fluid limit under the assumption that elastic scattering is the dominant process in the evolution (slow chemical reaction). All numerical values used in the simulations are to be considered as dimensionless; they have been chosen from existing literature (see e.g. Ref. 14 and Ref. 15), for illustrative and comparison purposes.

We consider two examples of Riemann problem with initial data reproducing macroscopic field such that $u_L = u_R = 0$, $\rho_L > \rho_R$, $T_L > T_R$. In both cases the structure of the exact solution for the inert case exhibits a shock wave propagating to the right, a contact shock wave propagating to the right and a rarefaction wave front moving to the left.¹⁶ When chemical reactions are taken into account, the solution can be found only numerically and its structure resembles the one of the corresponding inert problem.¹⁶

Test 1. In this first numerical test we consider a mixture of four gases having the following different values of masses $m_1 = 0.018$, $m_2 = 0.001$, $m_3 = 0.017$, $m_4 = 0.002$; the symmetric matrix \mathcal{N} of collision frequencies for elastic scattering for $k = 0$ is

$$\mathcal{N} = \begin{bmatrix} \nu_0^{11} = 5 & \nu_0^{12} = 6 & \nu_0^{13} = 2 & \nu_0^{14} = 7 \\ & \nu_0^{22} = 4 & \nu_0^{23} = 5 & \nu_0^{24} = 8 \\ & & \nu_0^{33} = 4 & \nu_0^{34} = 3 \\ & & & \nu_0^{44} = 6 \end{bmatrix} \quad (16)$$

and $\nu_1^{sr} = \nu_0^{sr}$ for $s, r = 1, \dots, 4$. The initial data $\underline{\phi}_0^s$ are chosen as Maxwellians reproducing prescribed global mass density ρ_0 , mean velocity u_0 and scalar pressure p_0 . Correspondingly, the initial mass density, mean velocity and scalar pressure for the four gases are

$$(\rho_0, u_0, p_0) = \begin{cases} \rho_{01} = 1.08 & \rho_{02} = 0.05 & \rho_{03} = 2.55 & \rho_{04} = 0.2 \\ u_{0i} = 0, & i = 1, \dots, 4, & p_0 = 2690 & \\ & & & x \leq 0, \\ \rho_{01} = 0.54 & \rho_{02} = 0.02 & \rho_{03} = 1.7 & \rho_{04} = 0.1, \\ u_{0i} = 0, & i = 1, \dots, 4, & p_0 = 500 & \\ & & & x > 0. \end{cases} \quad (17)$$

In this example we consider different values for the chemical collision frequency ν_{12}^{34} , defined in Ref. 6, and for the energy gap ΔE .

We began with the choice $\Delta E = 0$, which represents an important test for the consistency of our BGK model and of the relevant numerical approximation. It is known in fact that, starting from the reactive Boltzmann equations which our BGK model originated from, it is possible to derive, in the hydrodynamic limit, reactive Euler equations as zero order asymptotic approximation.⁵ It is remarkable that, when $\Delta E = 0$, this system gives the classical Euler equations for global mass densities, mean velocity and temperature, whereas the single mass densities ρ_i may differ from the inert case. Numerical results shown below in Figure 1 at time $t = 0.015$ for global density and global mean velocity confirm this behavior also when we start from the BGK model and approach the fluid limit under the same assumption of dominant elastic scattering (the same happens to temperature, not reported here). The computational domain in space and velocity is: $[-1, 1] \times [-500, 500]$. Numerical computations were carried out until the final time instant $t = 0.015$ with $(\Delta t, \Delta x, \Delta v) = (10^{-5}, 10^{-2}, 5)$. Knudsen number is $\varepsilon = 10^{-1}$. Simulations have been performed using both CSM

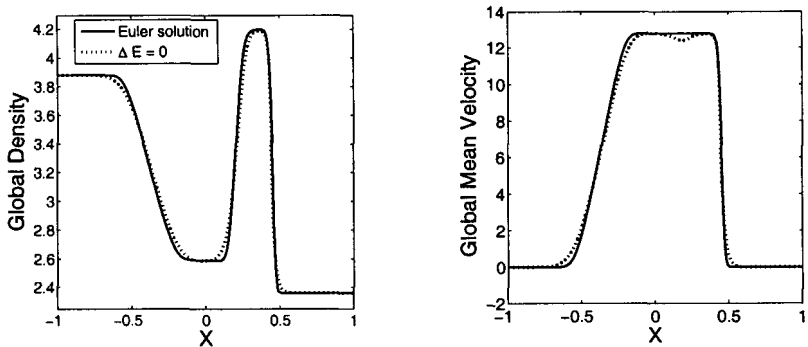


Fig. 1. Test of consistency for the reactive BGK model (with $\Delta E = 0$ at time $t = 0.015$).

coupled with Euler method and splitting (13) coupled with Heun method for the numerical solution of the collision steps. The variations of the profiles of the global density and global temperature for different values of the chemical collision frequency are shown in Figure 2 and for different values ΔE of energy difference between reactants and products are shown in Figure 3. We can notice that, in this example, the temperature increases either when the chemical reaction is faster or when ΔE is higher.

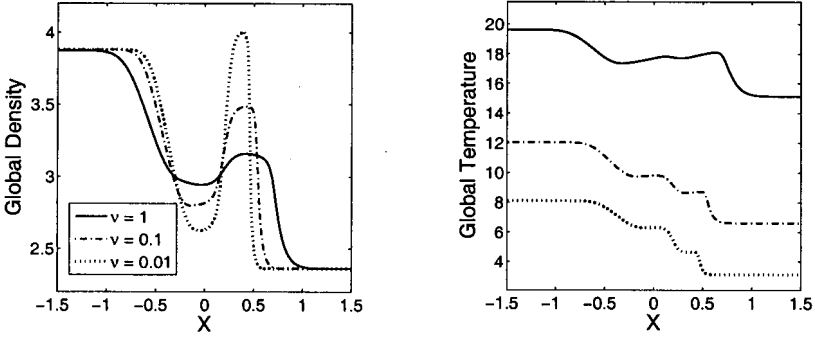


Fig. 2. Global density and global temperature for $\Delta E = 100$ at time $t = 0.015$ for different values of chemical collision frequency ν_{12}^{34} .

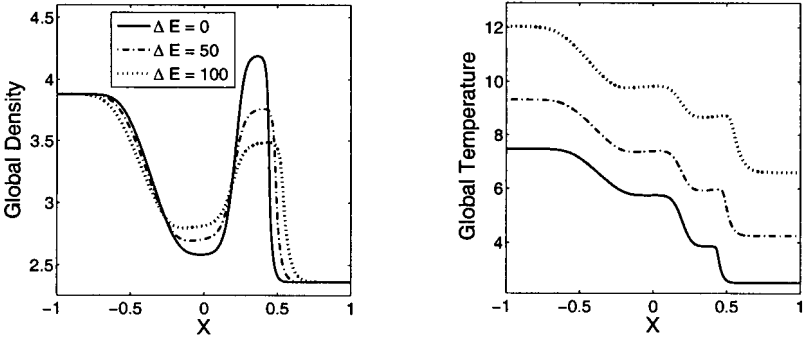


Fig. 3. Global density and global temperature for $\nu_{12}^{34} = 0.1$ at time $t = 0.015$ for different values of ΔE .

Test 2. In this second numerical test we consider a different mixture of four gases having the following different values of masses $m_1 = 58.5$, $m_2 = 18$, $m_3 = 40$, $m_4 = 36.5$, and the new symmetric matrix of collision frequencies for elastic scattering for $k = 0$ is $10^2 \mathcal{N}$, where \mathcal{N} is the matrix (16). The initial mass density, mean velocity and scalar pressure for the four gases are

$$(\rho_0, u_0, p_0) = \begin{cases} \rho_{0i} = \frac{i}{10}, u_{0i} = 0, i = 1, \dots, 4, p_0 = \frac{5}{3} & x \leq 0.5, \\ \rho_{0i} = \frac{i}{80}, u_{0i} = 0, i = 1, \dots, 4, p_0 = \frac{1}{6} & x > 0.5. \end{cases} \quad (18)$$

These initial data reproduce the classical Sod problem¹⁷ for Euler equations. The computational domain in space and velocity is: $[-0.5, 1.5] \times [-15, 15]$. Numerical computations were carried out until the final time instant $t = 0.2$ with $(\Delta t, \Delta x, \Delta v) = (5 \cdot 10^{-4}, 5 \cdot 10^{-3}, 5 \cdot 10^{-2})$. Knudsen number is $\varepsilon = 10^{-2}$. In this test we set the chemical collision frequency $\nu_{12}^{34} = 100$ and we consider different values of the energy gap ΔE . Simulations have been per-

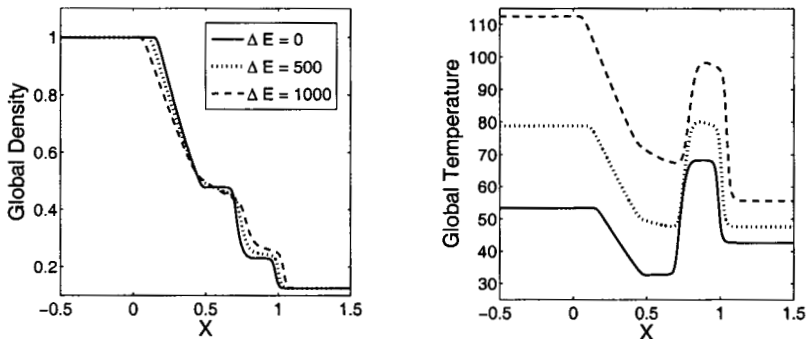


Fig. 4. Global density and global temperature at time instant $t = 0.2$ for different values of ΔE .

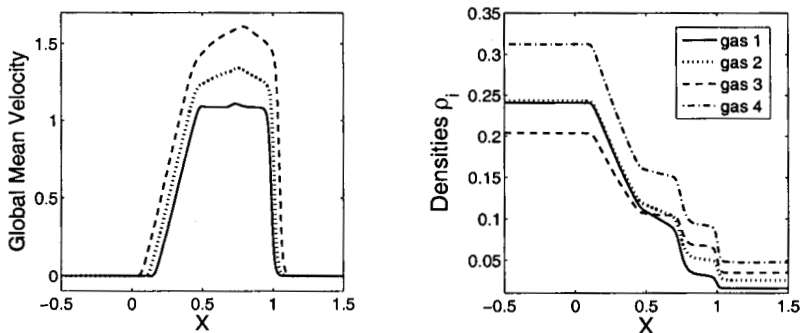


Fig. 5. Global mean velocity for different values of ΔE and densities $\rho_i, i = 1, \dots, 4$ for $\Delta E = 500$ at time instant $t = 0.2$.

formed using splitting (13) coupled with Heun method for the numerical solution of the collision steps. The variations of the profiles of global density ρ , global temperature T and global mean velocity u for different values ΔE at time instant $t = 0.2$ are shown in Figure 4 and in Figure 5 (left). In Figure 5 (right) we report the profiles of densities $\rho_i, i = 1, \dots, 4$, at the same time instant, for $\Delta E = 500$. The global moments of the inert mixture overlap the profiles obtained for $\Delta E = 0$, whereas this is not true

for the single components of the mixture. The higher ΔE , the greater the variations with respect to the inert case.

We notice moreover that the data used in Test 2 give rise to solutions in which the structure of density ρ and temperature T are somehow reversed with respect to Test 1.

References

1. I. Prigogine and E. Xhrouet, On the perturbation of Maxwell distribution function by chemical reaction in gases, *Physica* **XV**, 913 (1949).
2. V. Giovangigli, *Multicomponent Flow Modeling* (Birkhäuser, Boston, 1999).
3. P.L. Bhatnagar, E.P. Gross and K. Krook, A model for collision processes in gases, *Phys. Rev.* **94**, 511 (1954).
4. P. Welander, On the temperature jump in a rarefied gas, *Ark. Fys.* **7**, 507 (1954).
5. A. Rossani and G. Spiga, A note on the kinetic theory of chemically reacting gases, *Physica A* **272**, 563 (1999).
6. M. Groppi and G. Spiga, A Bhatnagar–Gross–Krook–type approach for chemically reacting gas mixtures, *Physics of Fluids* **16**, 4273 (2004).
7. Y. Sone, *Kinetic Theory and Fluid Dynamics* (Birkhäuser Verlag, Boston, 2002).
8. A.V. Bobylev and T. Ohwada, On the generalization of Strang’s splitting scheme, *Riv. Mat. Univ. Parma* (**6**) **2***, 235 (1999).
9. F. Filbet and G. Russo, High order numerical methods for the space non-homogeneous Boltzmann equation, *J. Comp. Phys.* **186**, 457 (2003).
10. T. Ohwada, Higher order approximation methods for the Boltzmann equation, *J. Comp. Phys.* **139**, 1 (1998).
11. C.K. Chu, Kinetic-theoretic description of the formation of a shock wave, *Phys. Fluids* **8**, 12 (1965).
12. M. Bisi, M. Groppi and G. Spiga, Grad’s distribution functions in the kinetic equations for a chemical reaction, *Continuum Mech. Thermodyn.* **14**, 207 (2002).
13. W.G. Bickley, Formulae for numerical differentiation, *Math. Gazette* **25**, 19 (1941).
14. C. Baranger and S. Pieraccini, Numerical simulation of models for reacting polytropic gases, in *”WASCOM 2005”–13th Conference on Waves and Stability in Continuous Media* (World Sci. Publ., Hackensack, NJ, 2006), 28.
15. M. Groppi and M. Pennacchio, An IMEX finite volume scheme for reactive Euler equations arising from kinetic theory, *Commun. Math. Sci.* **1**, 449 (2003).
16. F. Conforto, A. Jannelli, R. Monaco, T. Ruggeri, On the Riemann problem for a system of balance laws modelling a reactive gas mixture, *Physica A* **373**, 67 (2007).
17. G.A. Sod, A survey of several finite difference methods for systems of non-linear hyperbolic conservation laws, *J. Comput. Phys.* **27**, 1 (1978).