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On the shock thickness for a binary gas mixture

Marzia Bisi · Maria Groppi · Giorgio Martalò

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Abstract We discuss the structure of the shock wave solution for a system of Navier-Stokes equations, obtained as hydrodynamic limit of a BGK description of the dynamics of monoatomic gases at kinetic level. We investigate first the thickness of the transition region of the shock profile for a monoatomic gas, for varying Mach number and different physical options for the viscosity coefficient. The analysis is then extended to a binary gas mixture. Some numerical results for noble gases are presented and discussed.

Keywords Shock wave structure · Shock thickness · Navier-Stokes equations · BGK model

1 Introduction

Shock wave solutions for hyperbolic systems of conservation and balance laws have been widely studied [1–3], and the problem of the smoothness of such solutions has drawn a lot of attention [4–6].

More recently, many papers have been devoted to characterize global and piecewise smooth solutions in terms of singular barriers [7], especially in presence of multi-temperature models for gas mixtures [8–12].

In this paper, we focus on a particular feature of the shock wave structure concerning the shock thickness, i.e. the size of the narrow region where the transition from an equilibrium state to another occurs.

The thickness has order of magnitude of the mean free path of the particles and depends on the unperturbed Mach number, that characterizes the strength of the shock [13]. Although we expect the decrease of the thickness for increasing Mach number, experiments in monoatomic gases (some results for Argon

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are given in [14]) show that thickness decreases up to a certain Mach number (about 3.1 for Argon) and then increases again.

Some efforts to explain theoretically such behavior have been made starting from the classical paper of Gilbarg and Paolucci [15], where a continuum approach has been used, and also in the framework of general dissipative hyperbolic systems [13]. More specifically, in [15] it is also pointed out that a key role is played by viscosity and heat conductivity and the critical value for the Mach number strongly depends on these quantities.

In this paper, we investigate the shock thickness both for a single fluid and a binary mixture of monoatomic gases, whose evolutions are described by Navier-Stokes equations obtained as hydrodynamic limit of a recent BGK model [16, 17].

In particular, as regards the shock thickness for a single gas, we compare the results obtained with different models for viscosity (power laws and numerical approximation of experimental data given in [18]). As concerns the binary gas mixture, we model viscosity by suitable approximations of experimental values [18] and we discuss the occurrence of a possible critical value for Mach number, corresponding to a minimum for the shock thickness.

The paper is organized as follows: after recalling the kinetic BGK-type description for a binary gas mixture of monoatomic gases and its hydrodynamic closure at Navier-Stokes level in Section 2, we formulate the steady shock wave problem in Section 3 both for a single fluid and a binary mixture. In Section 4 we discuss the trend of shock thickness versus the unperturbed Mach number in both cases. Some concluding remarks are given in Section 5.

2 The mathematical model

2.1 Kinetic description

We consider a recent BGK-type description for a binary mixture of monoatomic gases [16] in a regime dominated by the elastic collisions [17]. The evolution of the distribution functions $f_i = f_i(\mathbf{x}, \boldsymbol{\xi}, t)$, $i = 1, 2$, is governed by the non-dimensional equations

$$\begin{aligned} \frac{\partial f_1}{\partial t} + \sum_{i=1}^3 \xi_i \frac{\partial f_1}{\partial x_i} &= \frac{1}{\varepsilon} [\nu_{11} (n_1 \mathcal{M}_{11} - f_1) + \nu_{12} (n_1 \mathcal{M}_{12} - f_1)] \\ \frac{\partial f_2}{\partial t} + \sum_{i=1}^3 \xi_i \frac{\partial f_2}{\partial x_i} &= \frac{1}{\varepsilon} [\nu_{21} (n_2 \mathcal{M}_{21} - f_2) + \nu_{22} (n_2 \mathcal{M}_{22} - f_2)] , \end{aligned} \quad (1)$$

where $\mathbf{x} \in \mathbb{R}^3$, $\boldsymbol{\xi} \in \mathbb{R}^3$, $t \in \mathbb{R}_+$ are position, microscopic velocity and time variable, respectively; $\varepsilon > 0$ is a small parameter corresponding to the Knudsen number, ν_{ij} , $i, j = 1, 2$, denotes the frequency of the collisions between components i and j . We remark that the i -th equation of this BGK model shows a sum of two relaxation operators, one describing collisions between particles

of i -th species, and the other counting for the effects on the i -th distribution function due to interactions with species $j \neq i$.

Each local attractor \mathcal{M}_{ij} , $i, j = 1, 2$, is a Maxwellian function

$$\mathcal{M}_{ij} = n_i \left(\frac{m_i}{2\pi T_{ij}} \right)^{\frac{3}{2}} \exp \left(-\frac{m_i}{2T_{ij}} |\boldsymbol{\xi} - \mathbf{u}_{ij}|^2 \right), \quad (2)$$

depending on the i -th particle mass m_i , species density n_i and some fictitious parameters \mathbf{u}_{ij} and T_{ij} . Such auxiliary quantities can be expressed in terms of the species macroscopic fields

$$\begin{aligned} n_i &= \int_{\mathbb{R}^3} f_i(\boldsymbol{\xi}) d\boldsymbol{\xi}, & \mathbf{u}_i &= \frac{1}{n_i} \int_{\mathbb{R}^3} \boldsymbol{\xi} f_i(\boldsymbol{\xi}) d\boldsymbol{\xi}, \\ 3n_i T_i &= m_i \int_{\mathbb{R}^3} |\boldsymbol{\xi} - \mathbf{u}_i|^2 f_i(\boldsymbol{\xi}) d\boldsymbol{\xi}, \end{aligned} \quad (3)$$

by imposing that the exchange rates for momentum and energy of each binary BGK operator coincide with the ones of the corresponding Boltzmann operator. This requirement automatically implies the correct conservation of global momentum and energy. These exchange rates can be made explicit for Maxwell molecules, and can be properly approximated for general intermolecular potentials. Specifically, one gets

$$\mathbf{u}_{ij} = (1 - a_{ij})\mathbf{u}_i + a_{ij}\mathbf{u}_j, \quad T_{ij} = (1 - b_{ij})T_i + b_{ij}T_j + \gamma_{ij}|\mathbf{u}_i - \mathbf{u}_j|^2, \quad (4)$$

with

$$\begin{aligned} a_{ij} &= \frac{\eta_{ij} n_i n_j}{\nu_{ij} (m_i + m_j)}, & b_{ij} &= \frac{2a_{ij} m_i}{m_i + m_j}, \\ \gamma_{ij} &= \frac{m_i a_{ij}}{3} \left(\frac{2m_j}{m_i + m_j} - a_{ij} \right), \end{aligned} \quad (5)$$

where η_{ij} is a suitable approximation of a proper averaged cross section and depends on the intermolecular potential. More precisely, ν_{ij} is constant for cross sections of Maxwell molecules type, while for general intermolecular potentials it is a non-constant function depending on species velocities and temperatures. As detailed in [16], a reasonable approximation is obtained by evaluating the averaged cross section in suitable points, leading to functions η_{ij} depending on $T_i, T_j, \mathbf{u}_i, \mathbf{u}_j$ through

$$z_{ij} = \left[3 \left(\frac{T_i}{m_i} + \frac{T_j}{m_j} \right) + |\mathbf{u}_i - \mathbf{u}_j|^2 \right]^{1/2}. \quad (6)$$

In order to guarantee the positivity of the global temperature, BGK collision frequencies must fulfill the constraints

$$\nu_{ij} \geq \frac{1}{2} \eta_{ij} n_j. \quad (7)$$

Proper choices of the BGK collision frequencies ν_{ij} are discussed in [16] again; here it is enough to point out that they may depend on number densities and on

averaged cross sections η_{ij} , and then possibly on other macroscopic moments of the distribution functions in case of interaction potentials different from Maxwell molecules.

A proper dissipation estimate has also been proved for such a BGK model [16], in terms of classical Boltzmann H -functional. Moreover, the indifferenciability principle holds, namely in a mixture of two identical gases, sharing of course the same mass, the distribution function $f_1 + f_2$ satisfies the BGK equation for a single monoatomic gas.

2.2 Hydrodynamic limit

We consider a first order expansion of the distribution functions

$$f_i = f_i^0 + \varepsilon f_i^1, \quad i = 1, 2, \quad (8)$$

and analogous expansions for the corresponding macroscopic quantities. As typical in Chapman-Enskog approximations, the macroscopic fields related to the collision invariants (namely n_i , \mathbf{u} , T) must be unexpanded.

By standard techniques, the following system of Navier-Stokes equations is obtained in the hydrodynamic limit (when $\varepsilon \rightarrow 0$)

$$\begin{aligned} \frac{\partial n_i}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_i \mathbf{u}) + \varepsilon \nabla_{\mathbf{x}} \cdot (n_i \mathbf{u}_i^1) &= 0, \quad i = 1, 2 \\ \frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} (nT) + \varepsilon \nabla_{\mathbf{x}} \cdot \mathbf{P}^1 &= \mathbf{0} \\ \frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \frac{3}{2} nT \right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho |\mathbf{u}|^2 + \frac{5}{2} nT \right) \mathbf{u} \right] \\ + \varepsilon \nabla_{\mathbf{x}} \cdot (\mathbf{P}^1 \cdot \mathbf{u}) + \varepsilon \nabla_{\mathbf{x}} \cdot \mathbf{q}^1 &= 0, \end{aligned} \quad (9)$$

where the corrections of order 1 (denoted by the superscript 1) for species mean velocities, global pressure tensor and heat flux are given respectively by [17]

$$\begin{aligned} \rho_1 \mathbf{u}_1^1 &= \frac{m_1 + m_2}{\eta_{12}^0} \frac{1}{\rho^2} [-m_2 n_2 \nabla_{\mathbf{x}} (n_1 T) + m_1 n_1 \nabla_{\mathbf{x}} (n_2 T)] = -\rho_2 \mathbf{u}_2^1 \\ P_{\ell m}^1 &= -T \left(\frac{n_1}{\nu_{11}^0 + \nu_{12}^0} + \frac{n_2}{\nu_{21}^0 + \nu_{22}^0} \right) \left(\frac{\partial u_\ell}{\partial x_m} + \frac{\partial u_m}{\partial x_\ell} - \frac{2}{3} \nabla_{\mathbf{x}} \cdot \mathbf{u} \delta_{\ell m} \right) \\ \mathbf{q}^1 &= \frac{5}{2} T (n_1 \mathbf{u}_1^1 + n_2 \mathbf{u}_2^1) \\ &\quad - \frac{5}{2} T \left(\frac{n_1}{m_1 (\nu_{11}^0 + \nu_{12}^0)} + \frac{n_2}{m_2 (\nu_{21}^0 + \nu_{22}^0)} \right) \nabla_{\mathbf{x}} T \end{aligned} \quad (10)$$

and

$$\begin{aligned} n &= n_1 + n_2, & \rho &= \rho_1 + \rho_2 = m_1 n_1 + m_2 n_2 \\ \rho \mathbf{u} &= \rho_1 \mathbf{u}_1 + \rho_2 \mathbf{u}_2, & T &= \frac{1}{n} \sum_{i=1}^2 n_i T_i + \frac{1}{3n} \sum_{i=1}^2 m_i n_i |\mathbf{u}_i - \mathbf{u}|^2. \end{aligned} \quad (11)$$

Terms ν_{ij}^0 ($i, j = 1, 2$) and η_{12}^0 are the zero order approximation of ν_{ij} and η_{12} , respectively. Their dependence on the macroscopic fields follows from the choice of BGK collision frequencies (as said above, see again [16]), taking into account that the macroscopic fields related to collision invariants (n_i , \mathbf{u} and T) must be unexpanded.

We can observe that \mathbf{P}^1 is a traceless tensor and it is proportional to the strain tensor via the viscosity coefficient

$$\mu = \left(\frac{n_1}{\nu_{11}^0 + \nu_{12}^0} + \frac{n_2}{\nu_{21}^0 + \nu_{22}^0} \right) T, \quad (12)$$

while the heat flux correction depends on the thermal conductivity coefficient

$$\lambda = \frac{5}{2} \left(\frac{n_1}{m_1(\nu_{11}^0 + \nu_{12}^0)} + \frac{n_2}{m_2(\nu_{21}^0 + \nu_{22}^0)} \right) T. \quad (13)$$

3 The steady shock wave problem

In this section we formulate the classical problem of the shock wave structure for the one dimensional steady version of the previous Navier-Stokes equations (9). We can get rid of the parameter ε by a proper scaling of the space variable, and substituting the relationships (10) in (9) we finally get

$$\begin{aligned} \frac{d}{dx}(n_i u) + (-1)^{i-1} \frac{d}{dx} \left\{ \frac{m_1 + m_2}{m_i} \frac{1}{\eta_{12}^0} \frac{1}{\rho^2} \times \right. \\ \left. \left[-m_2 n_2 \frac{d}{dx}(n_1 T) + m_1 n_1 \frac{d}{dx}(n_2 T) \right] \right\} = 0, \quad i = 1, 2 \\ \frac{d}{dx}(\rho u^2 + nT) - \frac{4}{3} \frac{d}{dx} \left(\mu \frac{du}{dx} \right) = 0 \\ \frac{d}{dx} \left[\left(\frac{1}{2} \rho u^2 + \frac{5}{2} nT \right) u \right] - \frac{4}{3} \frac{d}{dx} \left(\mu u \frac{du}{dx} \right) - \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) \\ + \frac{5}{2} \frac{d}{dx} \left\{ T(m_2 - m_1) \frac{m_1 + m_2}{m_1 m_2} \frac{1}{\eta_{12}^0} \frac{1}{\rho^2} \times \right. \\ \left. \left[-m_2 n_2 \frac{d}{dx}(n_1 T) + m_1 n_1 \frac{d}{dx}(n_2 T) \right] \right\} = 0, \end{aligned} \quad (14)$$

where the viscosity μ and thermal conductivity λ are given respectively in (12) and (13).

We observe that the first two equations in (14) give as expected the conservation of total mass

$$\frac{d}{dx}(\rho u) = 0, \quad (15)$$

and it can be used to express species density n_2 in terms of the remaining variables n_1 , u and T , reducing thus the number of equations.

The shock wave structure problem consists in discussing the solutions of (14) with asymptotic equilibrium condition at $\pm\infty$; we indicate such configurations by $E_{\pm} = (n_{1,\pm}, u_{\pm}, T_{\pm})$.

The analysis will be proposed for varying Mach number computed at $-\infty$

$$M^2 = \frac{3\rho_- u_-^2}{5n_- T_-}, \quad (16)$$

and the stationary state at $+\infty$ is connected to the equilibrium at $-\infty$ by means of classical Rankine-Hugoniot conditions

$$\begin{aligned} n_{1,+} &= \frac{4M^2}{M^2+3}n_{1,-}, & u_+ &= \frac{M^2+3}{4M^2}u_-, \\ T_+ &= \frac{(5M^2-1)(M^2+3)}{16M^2}T_-. \end{aligned} \quad (17)$$

Starting from the model for a binary gas mixture, thanks to the consistency properties of the model, it is possible to recover the hydrodynamic description for a single monoatomic gas by imposing that components share the same particle mass m ; more precisely, the system of differential equations (14) reduces to the well known steady Navier-Stokes equations [19, 20]

$$\begin{aligned} \frac{d}{dx}(\rho u) &= 0 \\ \frac{d}{dx}(\rho u^2 + nT) - \frac{4}{3} \frac{d}{dx} \left(\mu \frac{du}{dx} \right) &= 0 \\ \frac{d}{dx} \left[\left(\frac{1}{2}\rho u^2 + \frac{5}{2}nT \right) u \right] - \frac{4}{3} \frac{d}{dx} \left(\mu u \frac{du}{dx} \right) - \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) &= 0, \end{aligned} \quad (18)$$

where the viscosity and thermal conductivity coefficients obtained by the Chapman-Enskog procedure applied to the BGK model are given by

$$\mu = \frac{nT}{\nu^0}, \quad \lambda = \frac{5}{2} \frac{nT}{m\nu^0} = \frac{5}{2} \frac{\mu}{m}, \quad (19)$$

and ν^0 is the zero order approximation of the unique relaxation parameter that is involved at kinetic BGK level.

By using the conservation of mass (first equation in (18)), we have $\rho u = \text{const.}$, hence $\rho = \rho_- u_- / u$. By performing then analogous integrations in last two equations of (18), the system above can be reduced to two first order ODEs for the unknowns u and T , as

$$\begin{aligned} \frac{du}{dx} &= \frac{3}{4\mu} \left[\rho_- u_- (u - u_-) + n_- u_- \left(\frac{T}{u} - \frac{T_-}{u_-} \right) \right] \\ \frac{dT}{dx} &= -\frac{1}{2\lambda} \left[\rho_- u_- (u - u_-)^2 + n_- (5T_- u_- - 3T u_- - 2T_- u) \right]. \end{aligned} \quad (20)$$

The asymptotic states are given respectively by

$$E_- = (u_-, T_-), \quad E_+ = \left(\frac{M^2+3}{4M^2}u_-, \frac{(5M^2-1)(M^2+3)}{16M^2}T_- \right), \quad (21)$$

with $M^2 = (3mu_-^2)/(5T_-)$.

4 Analysis of shock thickness

We discuss the shock wave structure by investigating the rapid but continuous transition from an equilibrium state to another when $M > 1$. Its measure is usually given by the shock thickness [13,15]

$$\Delta = \frac{u_- - u_+}{\max |du/dx|}, \quad (22)$$

that clearly depends on the Mach number. In several papers [13–15], it has been pointed out that for monoatomic gases the thickness of the shock decreases up to a critical value for Mach number \hat{M} and then, in an unexpected way, it increases for higher values of Mach number.

After checking this result for a single gas with different intermolecular potentials, we analyze the shock thickness in a binary mixture of noble gases for varying Mach number.

4.1 Shock thickness for a single gas

In order to construct numerically the shock profile and hence evaluate the shock thickness, we first investigate the stability of equilibria at $\pm\infty$ by means of typical tools of the qualitative theory of dynamical systems.

We have that the jacobian matrix associated to (18) evaluated in E_-

$$\mathbf{J}_- = \mathbf{J}(E_-) = \begin{pmatrix} \frac{3n_-T_-}{4\mu(T_-)u_-} \left(\frac{5}{3}M^2 - 1 \right) & \frac{3n_-}{4\mu(T_-)} \\ \frac{n_-T_-}{\lambda(T_-)} & \frac{3n_-u_-}{2\lambda(T_-)} \end{pmatrix} \quad (23)$$

has two eigenvalues with positive real parts when $M > 1$, since

$$\begin{aligned} \det(\mathbf{J}_-) &= \frac{15}{8} \frac{n_-^2 T_-}{\mu(T_-)\lambda(T_-)} (M^2 - 1) > 0 \\ \text{tr}(\mathbf{J}_-) &= \frac{3n_-T_-}{4\mu(T_-)u_-} \left(\frac{5}{3}M^2 - 1 \right) + \frac{3n_-u_-}{2\lambda(T_-)} > 0. \end{aligned} \quad (24)$$

It is also possible to prove that eigenvalues are real [20]. Therefore, the equilibrium E_- is an unstable node with a two-dimensional unstable manifold.

As concerns the equilibrium state at $+\infty$, we have that the jacobian matrix evaluated in E_+

$$\mathbf{J}_+ = \mathbf{J}(E_+) = \begin{pmatrix} \frac{n_-T_-M^2}{2\mu(T_+)u_-(M^2+3)} (9 - 5M^2) & \frac{3n_-M^2}{\mu(T_+)(M^2+3)} \\ \frac{5n_-T_-(M^2-1)}{4\lambda(T_-)} & \frac{3n_-u_-}{2\lambda(T_+)} \end{pmatrix} \quad (25)$$

has negative determinant

$$\det(\mathbf{J}_+) = \frac{15}{2} \frac{n^2 T_-}{\mu(T_+) \lambda(T_+)} \frac{M^2}{M^2 + 3} (1 - M^2) < 0, \quad (26)$$

when $M > 1$; therefore, E_+ is a saddle point (then unstable) and both stable and unstable manifolds have dimension 1.

The shock solution, which can be viewed as the heteroclinic orbit connecting the two equilibria, is obtained numerically by a backward Runge-Kutta method, starting from a perturbation of equilibrium E_+ along the direction individuating the stable manifold.

It is clear that the shock structure strictly depends on the way we model viscosity (and hence thermal conductivity) [15]. In equation (19) we have observed that, in our derivation from the kinetic level, viscosity and thermal conductivity depend on the zero order approximation of the relaxation parameter ν^0 of the BGK description. By assuming that

$$\nu^0 = \sigma(T)n \quad (27)$$

then the function σ (and consequently the parameter ν^0) is uniquely determined as

$$\sigma(T) = \frac{T}{\mu(T)}. \quad (28)$$

In this analysis we consider and compare two different approximations for the viscosity $\mu(T)$:

1. a power law for temperature dependence of viscosity [19]

$$\mu = \mu_{\text{ref}} \left(\frac{T}{T_{\text{ref}}} \right)^k, \quad (29)$$

where T_{ref} is a reference temperature (we shall consider $T_{\text{ref}} = 50K$) and μ_{ref} is the corresponding value of viscosity for a chosen noble gas (see Table 1, where we report values for Argon and Helium). As concerns the parameter k , we consider

- a. $k = \frac{1}{2}$ corresponding to hard sphere intermolecular potential;
 - b. $k = 1$ corresponding to Maxwell molecule potential;
 - c. $k = \tilde{k}$ with $\frac{1}{2} < \tilde{k} < 1$ in order to reproduce a realistic potential (for example $\tilde{k} = 0.816$ for Argon and $\tilde{k} = 0.647$ for Helium) [15];
2. a least squares approximation (LSA) of the values of viscosity given in [18]; in particular we approximate the empirical values in the range $50 - 300K$ (see Table 1) by a linear function of the temperature

$$\mu = \alpha T + \beta, \quad (30)$$

where

- $\alpha = 0.0749$, $\beta = 0.6327$ for Argon;
- $\alpha = 0.0553$, $\beta = 3.8720$ for Helium.

	Argon	Helium
T (in K)	μ (in $\mu Pa \cdot s$)	μ (in $\mu Pa \cdot s$)
50	4.32	6.04
100	7.97	9.66
150	11.94	12.61
200	15.89	15.26
250	19.50	17.72
300	22.83	20.04

Table 1 Some experimental values of viscosity for Argon and Helium [18].

The thermal conductivity coefficient follows consequently from (19).

The profile of the shock thickness Δ versus the Mach number for Argon and Helium are reported in Figure 1 and 2, respectively. We observe that, when viscosity is modeled by power laws with exponent $k \neq 0.5$ or by the linear function (30), the shock thickness Δ decreases up to a critical value of the Mach number \hat{M} and then, from this value on, Δ increases. On the other hand, in the case of hard spheres intermolecular potential ($k = 0.5$ in the power law (29)), the shock thickness strictly decreases for increasing Mach numbers.

We notice also that the critical Mach number depends both on the chosen gas and on the viscosity model; more precisely, one has that

- for Argon $\hat{M}_{|k=1} \simeq 3.1 < \hat{M}_{|LSA} \simeq 3.4 < \hat{M}_{|k=\tilde{k}} \simeq 3.7$,
- for Helium $\hat{M}_{|k=1} \simeq 3.2 < \hat{M}_{|LSA} \simeq 4.2 < \hat{M}_{|k=\tilde{k}} \simeq 5.2$,

where $\hat{M}_{|k=1}$, $\hat{M}_{|k=\tilde{k}}$ and $\hat{M}_{|LSA}$ denote the critical Mach number when viscosity is described by a power law with exponent $k = 1$, a power law with exponent $k = \tilde{k}$ and a least square approximation, respectively.

We point out that when we consider a Maxwell molecules potential we obtain approximately the same critical value for the Mach number (around 3.1) for both gases, and such value is in agreement with the one obtained experimentally for Argon [14].

4.2 Shock thickness for a binary gas mixture

As done in the previous subsection, a preliminary analysis on the stability of asymptotic equilibria of system (14) for a binary mixture, which are

$$\begin{aligned}
 E_- &= (n_{1,-}, u_-, T_-) \\
 E_+ &= \left(\frac{4M^2}{M^2+3} n_{1,-}, \frac{M^2+3}{4M^2} u_-, \frac{(5M^2-1)(M^2+3)}{16M^2} T_- \right), \quad (31)
 \end{aligned}$$

provides some indications about the construction of the shock profiles.

As already shown in [21], for $M > 1$, the equilibrium E_- at $-\infty$ is unstable, with a three dimensional unstable manifold and no stable manifold; also the steady state E_+ at $+\infty$ is unstable, but with a two dimensional unstable

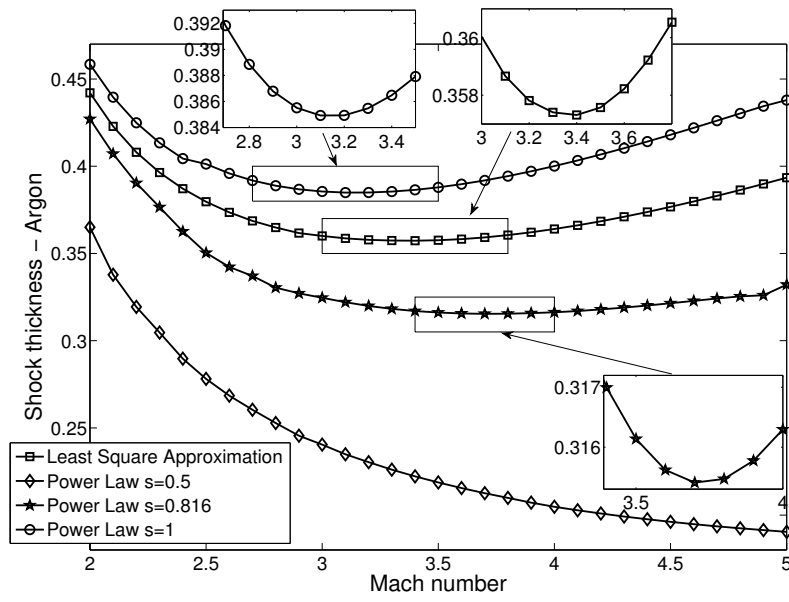


Fig. 1 Shock thickness Δ given in (22) versus Mach number for Argon and different models of viscosity and thermal conductivity.

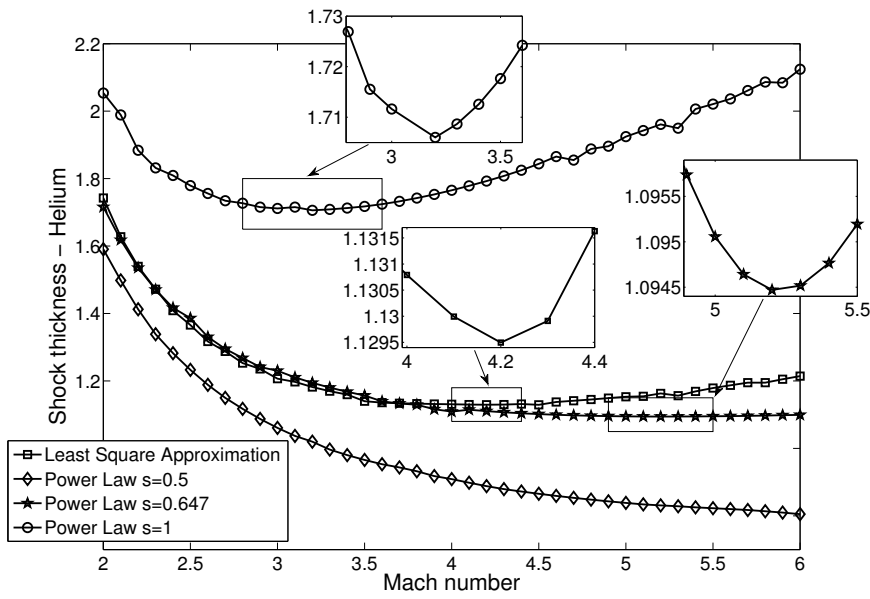


Fig. 2 Shock thickness Δ given in (22) versus Mach number for Helium and different models of viscosity and thermal conductivity.

and one dimensional stable manifolds, respectively. As in the case of a single gas, the shock profile is given by the heteroclinic orbit connecting the two equilibria and obtained numerically by solving backward with a Runge-Kutta scheme a Cauchy problem, with initial condition given by a perturbation of the equilibrium E_+ along the eigenvector corresponding to the stable manifold.

As concerns viscosity and thermal conductivity coefficients, we recall that their expressions consistently derived from our BGK model are given by (12) and (13), respectively; therefore, they are uniquely determined once the zero order approximations ν_{ij}^0 of the relaxation parameters ν_{ij} are given. Analogously to the case of a single gas, we assume that

$$\nu_{ij}^0 = \sigma_{ij}(T)n_j, \quad i, j = 1, 2, \quad (32)$$

and the symmetry relation $\sigma_{12} = \sigma_{21}$. Moreover, we denote by χ the concentration of the first component (and the concentration of the second species is therefore given by $1 - \chi$). It follows that viscosity and thermal conductivity coefficients given in (12) and (13) can be rewritten respectively as

$$\mu = \left(\frac{\chi}{\sigma_{11}\chi + \sigma_{12}(1 - \chi)} + \frac{1 - \chi}{\sigma_{12}\chi + \sigma_{22}(1 - \chi)} \right) T \quad (33)$$

and

$$\lambda = \frac{5}{2} \left(\frac{\chi}{m_1(\sigma_{11}\chi + \sigma_{12}(1 - \chi))} + \frac{1 - \chi}{m_2(\sigma_{12}\chi + \sigma_{22}(1 - \chi))} \right) T. \quad (34)$$

We observe that, in absence of the second component ($\chi = 1$), formula (33) should reproduce the viscosity of the first component as single fluid, and consequently the term σ_{11} is uniquely determined in terms of gas viscosity and temperature. Analogously, the quantity σ_{22} is determined by reproducing the viscosity of the second component as single gas, when $\chi = 0$.

In particular, for the i -th component, it follows that

$$\sigma_{ii} = \frac{T}{\mu_i}, \quad i = 1, 2, \quad (35)$$

where μ_i indicates the viscosity of the i -th species as single fluid. Some values of viscosity at certain reference temperatures are given in the first and second column of Table 2 for Neon and Argon. Using data of Table 2 (and for other noble gases see [18]) we obtain for such mixture some reference values for σ_{ii} by means of formula (35) and we approximate them linearly at any temperature by least squares method.

As concerns σ_{12} , we compute such quantity when the two components are equally concentrated ($\chi = 0.5$). In particular, from (33) we get that σ_{12} at a given temperature T is the positive solution of the quadratic algebraic equation

$$\mu\xi^2 + [\mu(\sigma_{11} + \sigma_{22}) - 2T]\xi + \mu\sigma_{11}\sigma_{22} - T(\sigma_{11} + \sigma_{22}) = 0, \quad (36)$$

where reference values of σ_{11} , σ_{22} are obtained as described above and values of viscosity at specific temperatures are given in the third column of Table 2

	$\chi = 1$	$\chi = 0$	$\chi = 0.5$
T (in K)	μ (in $\mu Pa \cdot s$)	μ (in $\mu Pa \cdot s$)	μ (in $\mu Pa \cdot s$)
50	7.70	4.32	5.68
100	14.39	7.97	9.90
150	19.72	11.94	13.76
200	24.29	15.89	17.57
250	28.36	19.50	21.44
300	32.10	22.83	25.32

Table 2 Some experimental values of viscosity for a mixture of Neon and Argon at different concentrations [18].

for a mixture of Neon and Argon. Some reference values of σ_{12} are obtained by solving equation (36) in correspondence of the tabulated temperatures and viscosities, and σ_{12} as function of a generic temperature T is deduced from a linear least squares approximation of these values. Heat conductivity follows consequently from equation (34).

For a mixture of Neon (first component) and Argon (second species), by means of the procedure described above, we obtain the following approximation for coefficients σ_{ij} , $i, j = 1, 2$,

$$\begin{aligned}
 \sigma_{11} &= 0.0117 T + 5.8587 \\
 \sigma_{12} &= 0.0084 T + 8.7089 \\
 \sigma_{22} &= 0.0050 T + 11.6710.
 \end{aligned}
 \tag{37}$$

Figure 3 shows the trend of the shock thickness Δ defined in (22) versus the Mach number for the considered mixture. We can notice that also for this binary mixture of monoatomic gases, the shock thickness rapidly decreases up to a critical value of the Mach number $\hat{M} \simeq 3.7$; then Δ increases from this value on.

Finally, in Figure 4 we can notice also that the critical Mach number depends on the chosen mixture and different choices of the concentrations lead to different critical Mach numbers. More precisely, the profile of the shock thickness versus the Mach number is shown for

- mixture of Neon (50%) and Argon (50%); critical value for Mach number $\hat{M} \simeq 3.9$ (see Panel (a));
- mixture of Krypton (50%) and Xenon (50%); critical value for Mach number $\hat{M} \simeq 3.6$ (see Panel (b));
- mixture of Neon (75%) and Argon (25%); critical value for Mach number $\hat{M} \simeq 4.3$ (see Panel (c));
- mixture of Krypton (75%) and Xenon (25%); critical value for Mach number $\hat{M} \simeq 3.5$ (see Panel (d)).

5 Conclusions

We have investigated the thickness of shock structure solutions for varying Mach number, when the fluid dynamic regime is modeled by a system of

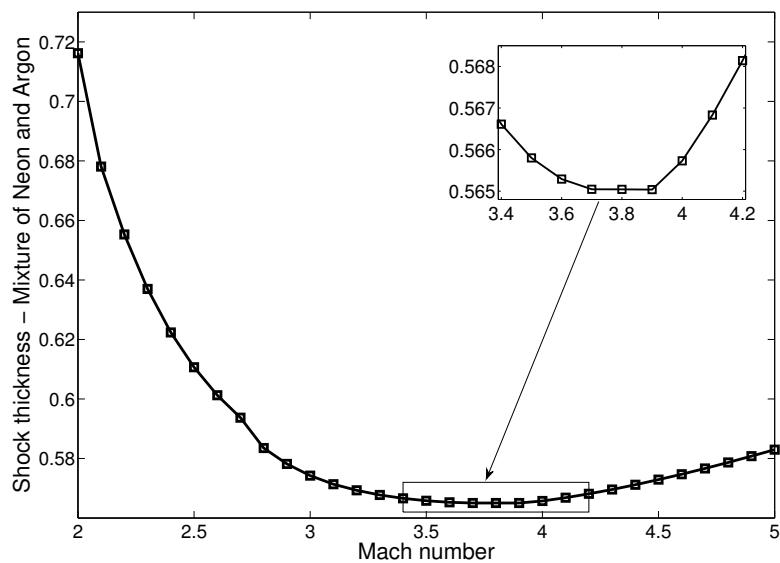


Fig. 3 Shock thickness Δ in (22) versus Mach number for a mixture of Neon (25%) and Argon (75%).

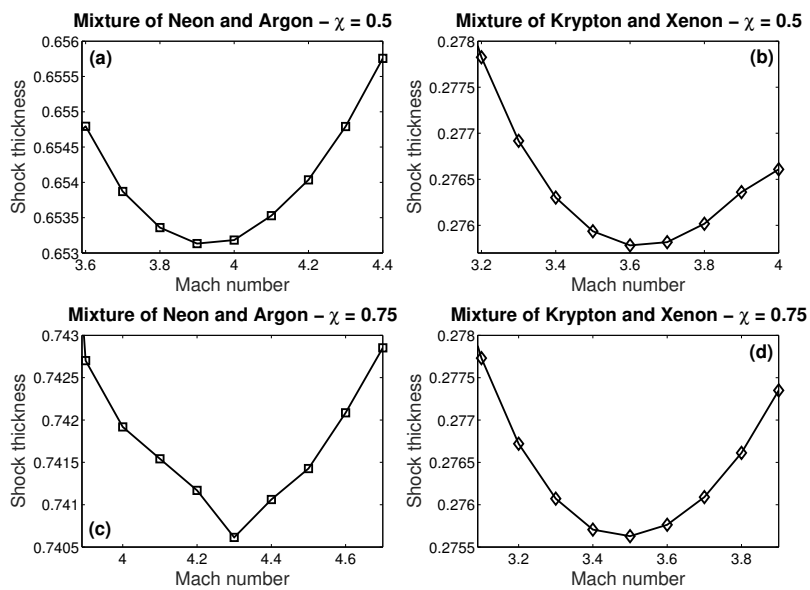


Fig. 4 Shock thickness Δ in (22) versus Mach number for mixtures of Neon and Argon and Krypton and Xenon at different concentrations.

Navier-Stokes equations consistently derived from a BGK model.

For a single gas, we have compared different models of viscosity and shown that in general the shock thickness is not monotonically decreasing for increasing Mach number. However, such behavior cannot be detected when the intermolecular potential of rigid spheres is considered.

We have shown, as already observed in experiments, the existence of a critical Mach number at which the shock thickness changes its trend, and a minimum shows up. We have noticed also that the value of such critical Mach number is strictly related to the chosen gas and viscosity model, in accordance with previous studies on shock thickness in single fluids.

The same analysis has been presented also for a binary mixture of monoatomic gases. To our knowledge, this issue has not yet been addressed in the literature (only partial results at fixed Mach number can be found for instance in [22–24]); here we take advantage also of the expression of viscosity coefficients obtained consistently by Chapman-Enskog asymptotics starting from a BGK model and fitted with real data. Our results show that also in the case of binary mixtures of noble gases the shock thickness is not strictly decreasing. As already observed in single fluids, a proper threshold for Mach number can be found for these mixtures and in correspondence of this value (depending on the chosen gaseous components of the mixture) the profile of shock thickness shows a minimum.

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Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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