

Two-fluid computational model for a binary gas mixture

Tatiana G. Elizarova^a, Irina A. Graur^a, Jean-Claude Lengrand^{b,*}

^a *Institute of Mathematical Modeling, Russian Academy of Sciences, Moscow, Russia*

^b *Laboratoire d'Aérodynamique du CNRS, Orléans, France*

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Abstract – This work is devoted to the derivation of moment equations for the description of a gasdynamic flow of a binary non-reacting gas mixture. The equations are based on the kinetic model in a relaxation approximation and they are a generalization of the quasigasdynamic equations studied before. As an example of applicability of the system proposed, we present calculations of flows in a shock wave for an argon-xenon mixture and of a binary diffusion problem for argon and helium, in comparison with the results of modeling these problems using the Direct Simulation Monte-Carlo method. A comparison with experimental results is also presented. © 2001 Éditions scientifiques et médicales Elsevier SAS

computational model / gas mixture / macroscopic equations

Nomenclature

a = speed of sound

\vec{c} = thermal speed

d = molecular diameter

E = total energy

f, F = distribution functions

k = Boltzmann constant

Kn = Knudsen number

Ma = Mach number

\mathcal{M} = molar mass

m = molecular mass

N = number of iterations

n = number density

Pr = Prandtl number

p = pressure

q = heat flux

R = perfect-gas constant per unit-mass

S = exchange terms

* Correspondence and reprints.

E-mail address: lengrand@cnrs-orleans.fr (J.-C. Lengrand).

T = temperature

t = time

\vec{u} = macroscopic velocity

γ = specific heat ratio

δ = shock wave thickness

λ = mean free path

μ = viscosity coefficient

ν = collision frequency

ρ = density

$\tau = \mu/p$, Maxwellian relaxation time

$\vec{\xi}$ = molecular velocity

ω = exponent in viscosity law

Subscripts and superscripts

1, 2 = conditions ahead of and behind the shock wave, respectively

a, b = gas species

ref = reference conditions

$(\bar{})$ ‘free parameters’

1. Introduction

The numerical simulation of gas-mixture flows is of great interest for both theoretical considerations and practical applications. An efficient simulation of non-reacting gas flows is a necessary step before developing models of gas flows with chemical reactions which in turn have a great practical directionality (e.g. [1]).

There are two groups of models for calculating gas-mixture flows. The first one consists of kinetic models, i.e. models based on direct numerical simulation methods (DSMC) or on the solution of the Boltzmann equation (e.g. [2]). The other group consists of macroscopic-equation systems which are derived on the basis of Navier–Stokes equations, in general by a phenomenological way, namely single-fluid and two-fluid models (e.g. [3, 4]).

The kinetic approximation offers an adequate gas-flow description but, as all kinetic models, has some disadvantages. In part, it loses its efficiency with decreasing Knudsen or Mach numbers. As for calculations, the moment methods are more efficient but the phenomenological ways of their derivation lead to a number of problems. These methods require the introduction of a number of additional constants, the determination of which is a separate problem.

In this paper we propose a new macroscopic model to describe flows of a binary non-reacting gas mixture. The model is a two-fluid approximation which is a system of equations for density, momentum and energy of each component. The system of macroscopic equations (named QGDM) is based on the kinetic equation in its relaxation approximation and is a natural generalization of the recently proposed quasigasdynamic (QGD) equations (e.g. [5–8]) for a gas mixture. Note that previously the QGD equations were generalized for gas flows in translational [9,10] and rotational [11,12] non-equilibrium.

2. Kinetic model

In 1954 Bhatnagar, Gross and Krook [13] published their famous equation (BGK) which is the Boltzmann equation with the collisional integral in its relaxation form. Though having a simple form, the model conserves the basic properties of the initial kinetic equation, therefore it has been applied widely to analyse a broad scope of problems. In 1962 Sirovich [14] gave a generalization of the BGK model for a gas mixture. In 1964 Morse [15], on the basis of the conservation relations, calculated the ‘free parameters’ missing before. In 1970 Wu and Lee [16] applied the kinetic model to calculate the one- dimensional flow of a binary mixture in a shock tube. In 1979 Platkowski [17] applied the mentioned model supplemented with Mott–Smith assumption to shock wave structure simulations. Those calculations were made for a gas with Prandtl number equal to unity $Pr = 1$, which is a consequence of the relaxation formulation in the initial kinetic model. Later some advanced kinetical models for a multicomponent gas were proposed (e.g. [18]).

We give a short description of the model according to [16].

Let the mixture consist of gas a and gas b with number densities n_a and n_b and accordingly with densities $\rho_a = m_a n_a$ and $\rho_b = m_b n_b$, where m_a and m_b are the masses of gas molecules a and b , respectively. Each gas is characterized by its temperature T_i and macroscopic velocity \vec{u}_i , where $i = a, b$. The perfect gas constant is $R_i = k/m_i$, where k is the Boltzmann constant.

Then according to [16] the kinetic model for the mixture can be expressed as

$$\frac{\partial f_a}{\partial t} + (\vec{\xi} \nabla) f_a = \nu_a (F_a - f_a) + \nu_{ab} (\bar{F}_a - f_a), \quad (1)$$

$$\frac{\partial f_b}{\partial t} + (\vec{\xi} \nabla) f_b = \nu_b (F_b - f_b) + \nu_{ba} (\bar{F}_b - f_b), \quad (2)$$

where $f_i(\vec{x}, \vec{\xi}, t)$ is the distribution function for species i , $\vec{\xi} = \vec{u} + \vec{c}$ is the molecule velocity, \vec{c} is the thermal velocity. ν_a and ν_b are the frequencies for self-collisions, ν_{ab} is the frequency for cross collisions of a molecules with b molecules and ν_{ba} is the frequency for cross collisions of b molecules with a molecules. The total number of collisions between species a and b should be balanced, so

$$n_a \nu_{ab} = n_b \nu_{ba}. \quad (3)$$

F_a , F_b and \bar{F}_a , \bar{F}_b are Maxwellian distribution functions defined as follows:

$$F_a = \frac{\rho_a}{(2\pi R_a T_a)^{3/2}} \exp\left(-\frac{(\vec{\xi} - \vec{u}_a)^2}{2R_a T_a}\right), \quad (4)$$

$$F_b = \frac{\rho_b}{(2\pi R_b T_b)^{3/2}} \exp\left(-\frac{(\vec{\xi} - \vec{u}_b)^2}{2R_b T_b}\right), \quad (5)$$

and

$$\bar{F}_a = \frac{\rho_a}{(2\pi R_a \bar{T}_a)^{3/2}} \exp\left(-\frac{(\vec{\xi} - \vec{\bar{u}}_a)^2}{2R_a \bar{T}_a}\right), \quad (6)$$

$$\bar{F}_b = \frac{\rho_b}{(2\pi R_b \bar{T}_b)^{3/2}} \exp\left(-\frac{(\vec{\xi} - \vec{\bar{u}}_b)^2}{2R_b \bar{T}_b}\right). \quad (7)$$

‘Free parameters’ (overlined) are present in formulas (4)–(7). According to [15], they can be related to gas parameters

$$\begin{aligned}\overline{\vec{u}_a} = \overline{\vec{u}_b} &= \frac{m_a \vec{u}_a + m_b \vec{u}_b}{m_a + m_b}, \\ \overline{T_a} &= T_a + \frac{2m_a m_b}{(m_a + m_b)^2} \left(T_b - T_a + \frac{m_b}{6k} (\vec{u}_b - \vec{u}_a)^2 \right), \\ \overline{T_b} &= T_b + \frac{2m_a m_b}{(m_a + m_b)^2} \left(T_a - T_b + \frac{m_a}{6k} (\vec{u}_b - \vec{u}_a)^2 \right).\end{aligned}\quad (8)$$

The distribution functions are interrelated and determine the macroscopic characteristics of the gas as

$$\int f_i d\vec{\xi} = \int F_i d\vec{\xi} = \int \bar{F}_i d\vec{\xi} = \rho_i, \quad (9)$$

$$\int \vec{\xi} f_i d\vec{\xi} = \int \vec{\xi} F_i d\vec{\xi} = \rho_i \vec{u}_i, \quad (10)$$

$$\int \vec{\xi} \bar{F}_i d\vec{\xi} = \rho_i \vec{u}_i, \quad (11)$$

$$\int \vec{c} f_i d\vec{\xi} = \int \vec{c} F_i d\vec{\xi} = \int \vec{c} \bar{F}_i d\vec{\xi} = 0, \quad (12)$$

$$\int \frac{\vec{\xi}^2}{2} f_i d\vec{\xi} = \int \frac{\vec{\xi}^2}{2} F_i d\vec{\xi} = \frac{\rho_i \vec{u}_i^2}{2} + \frac{3p_i}{2} = E_i, \quad (13)$$

$$\int \frac{\vec{\xi}^2}{2} \bar{F}_i d\vec{\xi} = \frac{\rho_i \vec{u}_i^2}{2} + \frac{3\bar{p}_i}{2} = \bar{E}_i. \quad (14)$$

Below this kinetic model is used by the authors to derive a system of macroscopic equations (QGDM) that describes the flow of a non-reactive binary mixture.

3. Macroscopic equations

Let us assume that the distribution functions for particles a and b are close to the corresponding local Maxwellian functions and can be represented approximately as gradient expansions in the vicinity of their equilibrium functions in the following form

$$f_a \rightarrow F_a - \tau (\vec{\xi} \nabla) F_a, \quad (15)$$

$$f_b \rightarrow F_b - \tau (\vec{\xi} \nabla) F_b. \quad (16)$$

Here τ is the Maxwellian relaxation time for the mixture. Its value is close to the mean time between collisions and it is defined as

$$\tau = \mu/p, \quad (17)$$

where μ is the mixture viscosity, p is the mixture pressure, equal to the sum of partial pressures, that is

$$p = p_a + p_b, \quad \text{where } p_a = \rho_a R_a T_a, \quad p_b = \rho_b R_b T_b. \quad (18)$$

The last two formulas are the partial equations of state.

We replace the true values of the distribution functions f_a, f_b in the convective terms of equations (1)–(2) by the (15)–(16) approximate values; then the kinetic model (1)–(2) is replaced by the approximate equations having the forms

$$\frac{\partial f_a}{\partial t} + \nabla_i \xi^i F_a - \nabla_i \tau \nabla_j \xi^i \xi^j F_a = \nu_a (F_a - f_a) + \nu_{ab} (\bar{F}_a - f_a), \quad (19)$$

$$\frac{\partial f_b}{\partial t} + \nabla_i \xi^i F_b - \nabla_i \tau \nabla_j \xi^i \xi^j F_b = \nu_b (F_b - f_b) + \nu_{ba} (\bar{F}_b - f_b). \quad (20)$$

Here subscripts i, j correspond to the space coordinates.

The macroscopic QGDM equations are derived by moment averaging of (19)–(20) over the velocity space ξ^i . To derive the macroscopic, or moment, equations we use the same method as was applied to derive the quasigasdynamic (QGD) equations for a one-component gas flow (see [10,12]). For both gases the systems of equations have the same form, so we describe the derivation procedure for gas a , omitting the subscript a .

Let us evaluate certain integrals useful for the future procedure.

$$\int c^i c^j F d\vec{\xi} = g^{ij} p, \quad (21)$$

where $g^{i,j}$ is the metric tensor.

$$\int c^i c^j c^k F d\vec{\xi} = 0, \quad (22)$$

$$\int c_x^4 F d\vec{\xi} = \int c_y^4 F d\vec{\xi} = \int c_z^4 F d\vec{\xi} = 3 \frac{p^2}{\rho}, \quad (23)$$

$$\int c_x^2 c_y^2 F d\vec{\xi} = \int c_x^2 c_z^2 F d\vec{\xi} = \int c_y^2 c_z^2 F d\vec{\xi} = \frac{p^2}{\rho}, \quad (24)$$

$$\int c^i c^j \bar{c}^2 F d\vec{\xi} = 5 \frac{p^2}{\rho} g^{ij}. \quad (25)$$

The limits of integration in all these integrals are infinite.

Integrating (19) with weight 1 and using (9), (12) and (21), we obtain

$$\int \frac{\partial f}{\partial t} d\vec{\xi} = \frac{\partial}{\partial t} \int f d\vec{\xi} = \frac{\partial}{\partial t} \rho;$$

$$\int \nabla_i \xi^i F d\vec{\xi} = \nabla_i \int (u^i + c^i) F d\vec{c} = \nabla_i \rho u^i;$$

$$\begin{aligned} \int \nabla_i \tau \nabla_j \xi^i \xi^j F d\vec{\xi} &= \nabla_i \tau \nabla_j \int (u^i + c^i)(u^j + c^j) F d\vec{c} \\ &= \nabla_i \tau \nabla_j \left(\rho u^i u^j + \int c^i c^j F d\vec{c} \right) \nabla_i \tau \nabla_j (\rho u^i u^j + g^{ij} p). \end{aligned}$$

As will be shown below the integral on the right-hand side of (19) vanishes.

Thus, we obtain the continuity equation in the form

$$\frac{\partial}{\partial t} \rho + \nabla_i \rho u^i = \nabla_i \tau \nabla_j (\rho u^i u^j + g^{ij} p). \quad (26)$$

To derive the momentum equation, we integrate (19) with weight ξ^k , using (10), (12), (21) and (22):

$$\begin{aligned} \int \frac{\partial f}{\partial t} \xi^k d\vec{\xi} &= \frac{\partial}{\partial t} \rho u^k, \\ \int \nabla_i \xi^i F \xi^k d\vec{\xi} &= \nabla_i (\rho u^i u^k + g^{ik} p), \\ \int \nabla_i \tau \nabla_j \xi^i \xi^j F \xi^k d\vec{\xi} &= \rho u^i u^j u^k + p(u^k g^{ij} + u^j g^{ik} + u^i g^{jk}). \end{aligned}$$

For the collision integral from equation (19) $\vec{\xi}$ is not a collisional invariant, because of momentum exchange between the species. Thus, the right-hand side integral does not vanish. It is called the exchange term and denoted here as S^u .

Combining the above relations yields the following equation for ρu^k :

$$\frac{\partial}{\partial t} \rho u^k + \nabla_i (\rho u^i u^k + g^{ik} p) = \nabla_i \tau \nabla_j [\rho u^i u^j u^k + p(u^k g^{ij} + u^j g^{ik} + u^i g^{jk})] + S^u. \quad (27)$$

To derive an equation for E , we average (19) with weight $\vec{\xi}^2/2$, using (9)–(14) and (21)–(25):

$$\begin{aligned} \int \frac{\partial f}{\partial t} \frac{\vec{\xi}^2}{2} d\vec{\xi} &= \frac{\partial}{\partial t} E, \\ \int \nabla_i \xi^i F \frac{1}{2} \vec{\xi}^2 d\vec{\xi} &= \nabla_i \frac{1}{2} \int (u^i + c^i) F \vec{\xi}^2 d\vec{c} = \nabla_i u^i (E + p), \\ \int \nabla_i \tau \nabla_j \xi^i \xi^j F \frac{\vec{\xi}^2}{2} d\vec{\xi} &= \nabla_i \tau \nabla_j \left(u^i u^j E + 2u^i u^j p + \frac{1}{2} u_k u^k g^{ij} p + \frac{5}{2} \frac{p^2}{\rho} g^{ij} \right). \end{aligned}$$

In this case also $\vec{\xi}^2/2$ is not a collisional invariant, because the species of the mixture may exchange energy. Thus, the last integral from equation (19) does not vanish. It is an exchange term denoted as S^E .

Combining these expressions and differentiating by parts the term containing the product of pressures, we obtain the following equation for energy:

$$\begin{aligned} \frac{\partial}{\partial t} E + \nabla_i u^i (E + p) &= \nabla_i \tau \nabla_j \left(u^i u^j E + 2u^i u^j p + \frac{1}{2} u_k u^k g^{ij} p \right) \\ &\quad + \frac{5}{2} \nabla_i \tau \frac{p}{\rho} \nabla_j p g^{ij} + \frac{5}{2} \nabla_i \tau p \nabla_j \frac{p}{\rho} g^{ij} + S^E. \end{aligned} \quad (28)$$

This method of deriving moment equations leads to expressions for the heat flux in which the Prandtl number is equal to unity. To extend the equations to the case of an arbitrary Prandtl number, the next to last term in the energy equation should be multiplied by Pr^{-1} .

The energy equation is derived here for a monoatomic gas, that corresponds to $\gamma = 5/3$. The generalization for the gases with internal (rotational) degrees of freedom was made in [11,12] and can be introduced by replacing the coefficient $5/3$ by γ in the energy expressions (13), (14) ($3p/2 \rightarrow p/(\gamma - 1)$) and in the last two terms of energy equation (28) ($5/2 \rightarrow \gamma/(\gamma - 1)$).

4. Calculation of exchange terms

The right-hand sides of the QGDM equations include exchange terms that are the moments of the collision integral, which arise when averaging over the molecular velocities. Using the relaxation model makes it possible to calculate those moments and to express them in terms of the gas macroparameters.

In the equation for density (19) the exchange terms are equal to zero. Indeed, the direct integration according to (9) gives

$$\begin{aligned} \int v_a (F_a - f_a) d\vec{\xi} &= v_a \left(\int F_a d\vec{\xi} - \int f_a d\vec{\xi} \right) = v_a (\rho_a - \rho_a) = 0, \\ \int v_{ab} (\bar{F}_a - f_a) d\vec{\xi} &= v_{ab} \left(\int \bar{F}_a d\vec{\xi} - \int f_a d\vec{\xi} \right) = v_{ab} (\rho_a - \rho_a) = 0. \end{aligned}$$

Integration with weight $\vec{\xi}$ when taking into account (10), (11) allows to calculate the exchange term in equation (27):

$$\begin{aligned} \int v_a (F_a - f_a) \vec{\xi} d\vec{\xi} &= v_a (\rho_a \vec{u}_a - \rho_a \vec{u}_a) = 0, \\ \int v_{ab} (\bar{F}_a - f_a) \vec{\xi} d\vec{\xi} &= v_{ab} (\rho_a \vec{u}_a - \rho_a \vec{u}_a) = S_a^u. \end{aligned}$$

In a similar manner, by averaging with weight $\vec{\xi}^2/2$, the exchange terms are calculated for the energy equation (28) when taking into account (12), (13)

$$\begin{aligned} \int v_a (F_a - f_a) \frac{\vec{\xi}^2}{2} d\vec{\xi} &= v_a (E_a - E_a) = 0, \\ \int v_{ab} (\bar{F}_a - f_a) \frac{\vec{\xi}^2}{2} d\vec{\xi} &= v_{ab} (\bar{E}_a - E_a) = S_a^E. \end{aligned}$$

For gases a and b the exchange terms have the form:

$$\begin{aligned} S_a^u &= v_{ab} \rho_a (\vec{u}_a - \vec{u}_a), & S_b^u &= v_{ba} \rho_b (\vec{u}_b - \vec{u}_b), \\ S_a^E &= v_{ab} (\bar{E}_a - E_a), & S_b^E &= v_{ba} (\bar{E}_b - E_b), \end{aligned} \quad (29)$$

respectively, where

$$\begin{aligned} \bar{E}_a &= (\rho_a \vec{u}_a^2)/2 + \bar{p}_a/(\gamma_a - 1), & \bar{p}_a &= \rho_a R_a \bar{T}_a, \\ \bar{E}_b &= (\rho_b \vec{u}_b^2)/2 + \bar{p}_b/(\gamma_b - 1), & \bar{p}_b &= \rho_b R_b \bar{T}_b. \end{aligned} \quad (30)$$

According to (3)

$$S_a'' + S_b'' = 0, \quad S_a^E + S_b^E = 0 \quad (31)$$

that coincides with momentum and energy conservation.

Thus, the QGDM model allows for an exchange of impulse and energy between the mixture components, the intensity of which is proportional to cross-collision frequencies between particles of different gases. There are no exchange terms in the equations for density, which is natural because the mixture components are supposed not to react with each other.

5. Determination of collision frequencies

To close the system of QGDM equations, it is necessary to estimate the cross-collision frequencies ν_{ab} and ν_{ba} and the relaxation time τ .

Relations between frequencies of collisions of a molecules with each other (self-collisions) and with b molecules (cross-collisions), according to [16], can be calculated in the following way:

$$\nu_{ab} = \nu_a \left(\frac{d_{ab}}{d_a} \right)^2 \sqrt{\frac{m_a + m_b}{2m_a m_b} \frac{n_a}{n_b}}, \quad (32)$$

here d_a is the effective molecular diameter for gas a , d_{ab} is the effective diameter which can be determined, for example, according to [2], p. 16, as $d_{ab} = 0.5(d_a + d_b)$. In turn, the collision frequency ν_a can be connected with the gas viscosity. In the approximation of the VHS and VSS models for particle interactions, this relationship has a form [2], p. 90:

$$\nu_a = \frac{p_a}{\mu_a} \Omega(\omega_a, \alpha_a), \quad \mu_a = \mu_{\text{aref}} \left(\frac{T_a}{T_{\text{aref}}} \right)^{\omega_a}, \quad \text{where } \Omega(\omega_a, \alpha_a) = \frac{5(\alpha_a + 1)(\alpha_a + 2)}{\alpha_a(7 - 2\omega_a)(5 - 2\omega_a)}. \quad (33)$$

For further calculations $\alpha_a = 1$ is used, that conforms to the VHS model ([2], p. 41). In this case we write $\Omega(\omega_a, 1) = \Omega(\omega_a)$.

The total number of collisions between molecules of gases a and b should be balanced, i.e. relation (3) must be satisfied. But the expressions for collision frequencies (32) and (33) comply with this balance relation in the only case of Maxwellian molecules ($\omega = 1$), when $T_{\text{aref}} = T_{\text{bref}}$. Thus, if one of the cross-collision frequencies is determined according to (32)–(33), then the other frequency should be determined from balance relation (3).

In equations (26), (27), (28) there is a parameter τ defined as the Maxwellian relaxation time for a mixture (17). To determine the binary-mixture viscosity, there is, for example, the Wilke formula [19]:

$$\mu = \mu_a \left(1 + G_{ab} \frac{\rho_b \mathcal{M}_a}{\rho_a \mathcal{M}_b} \right)^{-1} + \mu_b \left(1 + G_{ba} \frac{\rho_a \mathcal{M}_b}{\rho_b \mathcal{M}_a} \right)^{-1},$$

$$\text{where } G_{ab} = \frac{\left(1 + \sqrt{\mu_a / \mu_b \sqrt{\mathcal{M}_b / \mathcal{M}_a}} \right)^2}{2\sqrt{2}(1 + \mathcal{M}_a / \mathcal{M}_b)}, \quad (34)$$

here $\mathcal{M}_a, \mathcal{M}_b$ are the molar masses of gases a and b respectively.

Note, that the collision frequencies and the binary-mixture viscosity are parameters ‘external’ to the QGDM model and could be determined by other estimations. For example, other expressions exist for the frequency of cross-collisions (see, for example, [2], p. 96). Another expression for the binary-mixture viscosity is written in the book by Chapman and Cowling [20], p. 275 and in [3]. In [21] the viscosity coefficients of separate components are given.

6. Quasigasdynamic (QGDM) equations for a gas mixture

Raising indices in the resulting equations by means of the metric tensor we obtain the final QGDM equations for a binary gas mixture in a invariant form. For both gases the systems of equations have the same form and the system of equations, describing gas a , is written below:

$$\frac{\partial}{\partial t} \rho_a + \nabla_i \rho_a u_a^i - \nabla_i \tau (\nabla_j \rho_a u_a^i u_a^j + \nabla^i p_a) = 0, \quad (35)$$

$$\frac{\partial}{\partial t} \rho_a u_a^k + \nabla_i \rho_a u_a^i u_a^k + \nabla^k p_a = \nabla_i \tau (\nabla_j \rho_a u_a^i u_a^j u_a^k + \nabla^i p_a u_a^k + \nabla^k p_a u_a^i) + \nabla^k \tau \nabla_i p_a u_a^i + S_a^u, \quad (36)$$

$$\begin{aligned} \frac{\partial}{\partial t} E_a + \nabla_i u_a^i (E_a + p_a) = \nabla_i \tau \left(\nabla_j (E_a + 2p_a) u_a^i u_a^j + \frac{1}{2} \nabla^i u_{ak} u_a^k p_a \right) + \frac{\gamma_a}{\gamma_a - 1} \nabla_i \tau \frac{p_a}{\rho_a} \nabla^i p_a \\ + Pr_a^{-1} \frac{\gamma_a}{\gamma_a - 1} \nabla_i \tau p_a \nabla^i \frac{p_a}{\rho_a} + S_a^E, \end{aligned} \quad (37)$$

where the energy for gas a becomes

$$E_a = (\rho_a \vec{u}_a^2)/2 + p_a/(\gamma_a - 1). \quad (38)$$

The exchange terms are calculated as (29), (30), the ‘free parameters’ are calculated as (8), the frequencies of cross-collisions and the viscosity coefficient of the binary mixture can be found using (32), (33) and (34). When supplemented with boundary conditions, this set of equations constitutes a closed model for computing flows of a binary gas mixture in a two-fluid approach. It is much more simple than the two-fluid model for a gas mixture, as obtained by the Chapman–Enskog procedure [22].

The mixture parameters (no subscript) relate to the species parameters:

$$\begin{aligned} n &= n_a + n_b, & \rho &= \rho_a + \rho_b, & p &= p_a + p_b, & u &= (\rho_a u_a + \rho_b u_b)/\rho, \\ T &= (n_a T_a + n_b T_b)/n, & m &= (m_a n_a + m_b n_b)/n, & p &= \rho RT, \\ R &= (\rho_a R_a + \rho_b R_b)/\rho = k/m. \end{aligned} \quad (39)$$

For a single-component gas, the system (35)–(38) coincides with the QGD system investigated earlier (e.g. [6–8]). The relation between QGD and Navier–Stokes equations for a dilute gas was analysed in [7,8]. In particular, QGD equations were presented as balance equations for mass, momentum, and total energy in local form:

$$\frac{\partial}{\partial t} \rho + \nabla_i J^i = 0, \quad \frac{\partial}{\partial t} \rho u^k + \nabla_i J^i u^k = \nabla_i P^{ik}, \quad \frac{\partial}{\partial t} E + \nabla_i J^i \frac{E}{\rho} = \nabla_i (A^i - q^i). \quad (40)$$

Here

$$J^i = \rho u^i - \tau(\nabla_j \rho u^i u^j + \nabla^i p) \quad (41)$$

is the mass flux density. The stress tensor P^{ik} , the heat flux q^i , and the vectors J^i and A^i are sums of the corresponding variables in the Navier–Stokes representation with additional terms whose asymptotic order is $O(\tau^2)$ for steady flows if the bulk viscosity η in the Navier–Stokes model is approximated by the expression [10]

$$\eta = \mu(5/3 - \gamma), \quad \text{where } \mu = p\tau.$$

For a one-dimensional plane flow, the QGDM system simplifies and writes as

$$\frac{\partial \rho_a}{\partial t} + \frac{\partial}{\partial x} \rho_a u_a = \frac{\partial}{\partial x} \tau \frac{\partial}{\partial x} (\rho_a u_a^2 + p_a), \quad (42)$$

$$\frac{\partial \rho_b}{\partial t} + \frac{\partial}{\partial x} \rho_b u_b = \frac{\partial}{\partial x} \tau \frac{\partial}{\partial x} (\rho_b u_b^2 + p_b), \quad (43)$$

$$\frac{\partial \rho_a u_a}{\partial t} + \frac{\partial}{\partial x} (\rho_a u_a^2 + p_a) = \frac{\partial}{\partial x} \tau \frac{\partial}{\partial x} (\rho_a u_a^3 + 3p_a u_a) + S_a^u, \quad (44)$$

$$\frac{\partial \rho_b u_b}{\partial t} + \frac{\partial}{\partial x} (\rho_b u_b^2 + p_b) = \frac{\partial}{\partial x} \tau \frac{\partial}{\partial x} (\rho_b u_b^3 + 3p_b u_b) + S_b^u, \quad (45)$$

$$\begin{aligned} \frac{\partial E_a}{\partial t} + \frac{\partial}{\partial x} u_a (E_a + p_a) &= \frac{\partial}{\partial x} \tau \frac{\partial}{\partial x} u_a^2 (E_a + 2.5p_a) \\ &+ \frac{\gamma_a}{\gamma_a - 1} \frac{\partial}{\partial x} \tau \frac{p_a}{\rho_a} \frac{\partial p_a}{\partial x} + \frac{\gamma_a}{\gamma_a - 1} \frac{1}{Pr_a} \frac{\partial}{\partial x} \tau p_a \frac{\partial}{\partial x} \frac{p_a}{\rho_a} + S_a^E, \end{aligned} \quad (46)$$

$$\begin{aligned} \frac{\partial E_b}{\partial t} + \frac{\partial}{\partial x} u_b (E_b + p_b) &= \frac{\partial}{\partial x} \tau \frac{\partial}{\partial x} u_b^2 (E_b + 2.5p_b) \\ &+ \frac{\gamma_b}{\gamma_b - 1} \frac{\partial}{\partial x} \tau \frac{p_b}{\rho_b} \frac{\partial p_b}{\partial x} + \frac{\gamma_b}{\gamma_b - 1} \frac{1}{Pr_b} \frac{\partial}{\partial x} \tau p_b \frac{\partial}{\partial x} \frac{p_b}{\rho_b} + S_b^E. \end{aligned} \quad (47)$$

This equation system will be used further for the numerical simulation of binary gas mixtures.

7. Shock wave structure in a helium–xenon mixture

As a first example of using the QGDM equations we considered the problem of a stationary shock wave structure in a mixture of helium (He is gas a) and xenon (Xe is gas b). Density profiles for these gases, measured with the use of an electron gun and a laser interferometer, can be found in [23]. Measurements were performed for the following variants:

- variant V1 – 98.5% He and 1.5% Xe;
- variant V2 – 97% He and 3% Xe;
- variant V3 – 94% He and 6% Xe;
- variant V4 – 91% He and 9% Xe.

For variant V2, there is a calculation by the DSMC method [2], the results of which can be considered as a reference.

Table I presents the parameters of the mixture before the shock wave, chosen in accordance with the experimental data from [23] and with the calculation from [2]. In *table II* are physical parameters of helium and xenon according to [2], which are necessary to perform calculations by the QGDM model. The Prandtl number for the gases is constant and equal to $Pr = 2/3$.

The system of equations (42)–(47) is solved in non-dimensional variables taking as dimensional scales the following characteristics of gas a in the upstream flow: $\rho_{a\text{ref}}$ is the density, $a_{a\text{ref}} = \sqrt{\gamma_a R_a T_{a\text{ref}}}$ is the sound velocity at temperature $T_{a\text{ref}}$, $\lambda_{a\text{ref}}$ is the mean free path, that is computed as in [2]:

$$\lambda = \frac{4\mu}{\rho\sqrt{RT}} \frac{1}{\sqrt{2\pi}\Omega(\omega)}. \quad (48)$$

Then relations between the dimensional and dimensionless parameters have the following forms (all parameters of gas b are scaled by parameters of gas a):

$$\rho = \tilde{\rho}\rho_{a\text{ref}}, \quad a = \tilde{a}a_{a\text{ref}}, \quad u = \tilde{u}a_{a\text{ref}}, \quad p = \tilde{p}\rho_{a\text{ref}}a_{a\text{ref}}^2, \quad m = \tilde{m}\rho_{a\text{ref}}\lambda_{a\text{ref}}^3,$$

$$T = \tilde{T} \frac{a_{a\text{ref}}^2}{\gamma_a R_a} = \tilde{T} T_{a\text{ref}}, \quad x = \tilde{x}\lambda_{a\text{ref}}, \quad t = \tilde{t} \frac{\lambda_{a\text{ref}}}{a_{a\text{ref}}}, \quad n = \tilde{n} \frac{1}{\lambda_{a\text{ref}}^3}.$$

Equations (42)–(47) do not change their forms after the process of scaling. The relations between the parameters of the gases (link equations) become

$$\tilde{a}_a = \sqrt{\tilde{T}_a}, \quad \tilde{a}_b = \sqrt{\frac{\gamma_b R_b}{\gamma_a R_a} \tilde{T}_b}, \quad \tilde{T}_a = \frac{\gamma_a \tilde{p}_a}{\tilde{\rho}_a}, \quad \tilde{T}_b = \frac{\gamma_a \tilde{p}_b R_a}{\tilde{\rho}_b R_b},$$

$$\tilde{\mu}_a = \tilde{T}_a^{\omega_a}, \quad \tilde{\mu}_b = \frac{\mu_{b\text{ref}}}{\mu_{a\text{ref}}} \left(\frac{T_{a\text{ref}}}{T_{b\text{ref}}} \right)^{\omega_b} \tilde{T}_b^{\omega_b},$$

here $\mu_{b\text{ref}}$ and $T_{b\text{ref}}$ are the viscosity coefficient and the corresponding temperature of gas b , used in the viscosity-law (33).

In *table III* are values of the non-dimensional parameters in the upstream gas flow for variant V2.

The boundary conditions on the right and left boundaries were taken from the Rankine–Hugoniot conditions for a stationary shock wave in a gas mixture. The variables on the right of the discontinuity are computed as follows

$$\rho_2 = \rho_1 \frac{(\gamma + 1)Ma^2}{2 + (\gamma - 1)Ma^2}, \quad p_2 = p_1 \frac{2\gamma Ma^2 - \gamma + 1}{\gamma + 1}, \quad u_2 = u_1 \frac{2 + (\gamma - 1)Ma^2}{(\gamma + 1)Ma^2}, \quad (49)$$

where subscripts 1 and 2 refer to Rankine–Hugoniot conditions upstream (1) and downstream (2) of the shock wave. The component temperatures are found from the state equations.

Assume that the temperatures and velocities of the components before and after the shock wave are equal, and the mass-fraction of the components after the transition through the shock are unchanged. Thus on the basis of conditions (49), the parameters of each component of the mixture are derived from the ratios:

$$\begin{aligned} \rho_{a1}/\rho_{b1} &= \rho_{a2}/\rho_{b2}, & T_{a1} &= T_{b1} = T_1, & u_{a1} &= u_{b1} = u_1, \\ T_{a2} &= T_{b2} = T_2, & u_{a2} &= u_{b2} = u_2. \end{aligned}$$

(50)

The initial conditions are a discontinuity at point $x = 0$:

$$\begin{aligned} \text{at } x \leq 0 \quad & \rho_a = \rho_{a1}, \quad \rho_b = \rho_{b1}, \quad T_a = T_b = T_1, \quad u_a = u_b = u_1; \\ \text{at } x \geq 0 \quad & \rho_a = \rho_{a2}, \quad \rho_b = \rho_{b2}, \quad T_a = T_b = T_2, \quad u_a = u_b = u_2. \end{aligned}$$

(51)

The same quantities are used as boundary conditions.

Table I. Dimensional parameters of mixture components for variants V1 to V4.

	V1		V2		V3		V4	
	He	Xe	He	Xe	He	Xe	He	Xe
$\rho \text{ (kg/m}^3\text{)} \cdot 10^5$	5.15	2.57	5.16	2.22	4.91	10.3	4.57	14.8
$p \text{ (Pa)}$	33.14	0.51	33.21	1.02	31.62	2.02	29.42	2.91
$T \text{ (K)}$	310.							
$u \text{ (m/s)}$	3076.76		2882.6		2672.8		2530.3	
Ma	2.97	17.01	2.78	15.93	2.58	14.78	2.44	13.99

Table II. Tabulated values for mixture components.

	He	Xe
$m \text{ (kg)}$	$6.65 \cdot 10^{-27}$	$218 \cdot 10^{-27}$
$R \text{ (J/(kg} \cdot \text{K))}$	2076.2	63.33
$\mathcal{M} \text{ (kg/mol)}$	4.0	131.4
$d \text{ (m)}$	$2.30 \cdot 10^{-10}$	$5.65 \cdot 10^{-10}$
γ	1.66	1.66
ω	0.66	0.85
$\mu_{\text{ref}} \text{ (N/(m} \cdot \text{s)) at } T = 273 \text{ K}$	$2.03 \cdot 10^{-5}$	$2.34 \cdot 10^{-5}$

Table III. Non-dimensional parameters for variant V2.

	Gas a (He)	Gas b (Xe)	Mixture
ρ	1.	1.011	2.011
T	1.	1.	1.
a	1.	0.175	0.715
λ	1.	5.485	1.134
p	0.6	0.0185	0.618
Ma	2.78	15.93	3.89

Table IV. Calculation parameters for variant V2.

	Grid 601	Grid 1201
Grid step h	0.5	0.25
Time step Δt	$4.8 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$
Number of iterations N_{iter}	90251	360450

To solve the (42)–(47) system, an explicit difference scheme was applied where the steady-state solution was obtained as the limit of a time-evolving process. All spatial derivatives, including the convective terms, were approximated by central differences (see, for instance, [10,12]).

The problem was solved using a uniform spatial grid with a convergence criterion $\varepsilon_{\rho a} = 10^{-5}$. When refining the grid by a factor of 2 and 4, the differences between the computational results were extremely small, which allows to conclude that grid convergence has been reached. As an example, the parameters of numerical computation for variant V2 are presented in *table IV*.

The profiles of gas-dynamic parameters (those of velocity, density, temperature) are given in a normalized form on the basis of upstream and downstream Rankine–Hugoniot conditions. In this case, $\rho \rightarrow (\rho - \rho_1)/(\rho_2 - \rho_1)$; similarly for the temperature. For the velocity $u \rightarrow (u - u_2)/(u_1 - u_2)$.

Let the computational results for variant V2 be considered in detail. In *figures 1 to 5* the profiles of gasdynamic parameters at the shock-wave front are shown in comparison with the corresponding results

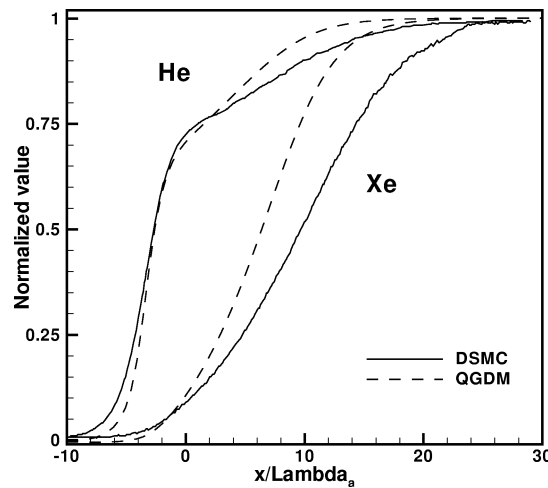


Figure 1. Density profiles in a He–Xe mixture.

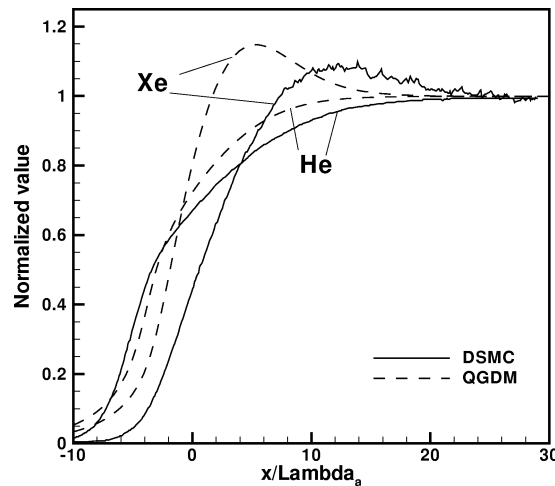


Figure 2. Temperature profiles in a He–Xe mixture.

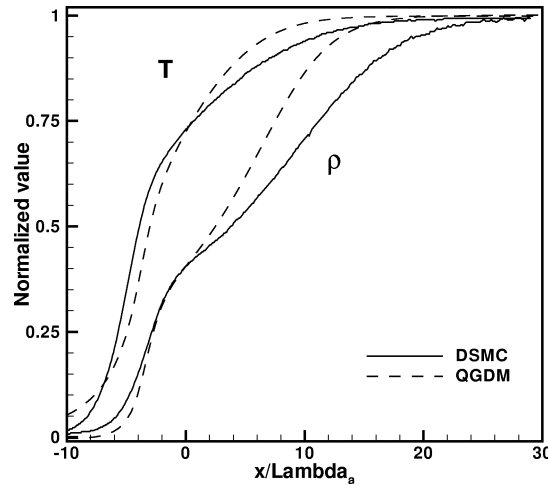


Figure 3. Mean temperature and density profiles in a He–Xe mixture.

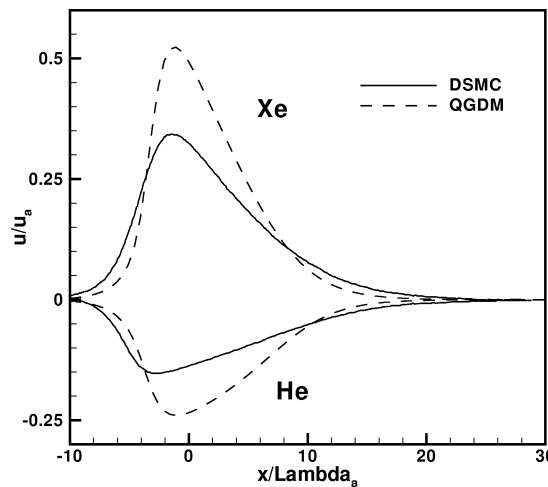


Figure 4. Diffusion velocities in a shock wave.

obtained in [2] on the basis of the DSMC method. The curves, corresponding to the DSMC calculations, are superimposed on the QGDM data, so that the values of the mean density be coincide at $x = 0$.

Figures 1 and 2 show the profiles of density and temperature of helium and xenon. The distributions of the mean density and temperature for the mixture are given in figure 3. Like in the DSMC model, the temperature of xenon overshoots its final value by $\sim 10\%$ and the mean mixture temperature is close to the helium temperature.

In figure 4 are presented the diffusion velocities u_{da} and u_{db} , reduced by the upstream flow velocity.

$$u_{da} = u_a - u, \quad u_{db} = u_b - u. \quad (52)$$

In figure 5 the xenon concentration is presented. Within the shock wave, it falls to approximately half its initial value.

The curves demonstrate that the QGDM model reflects at least qualitatively the main features of the flow.

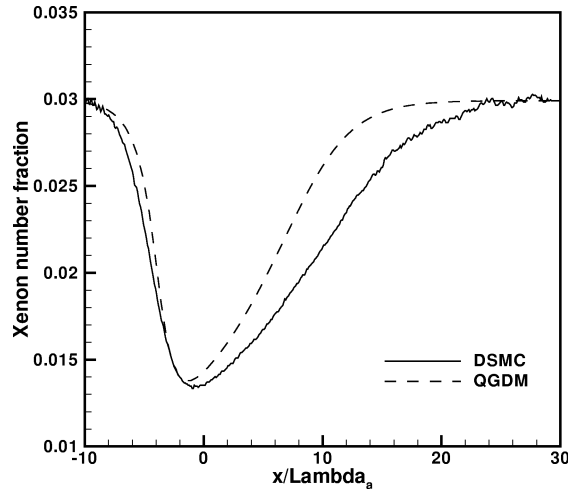


Figure 5. Xenon concentration in a shock wave.

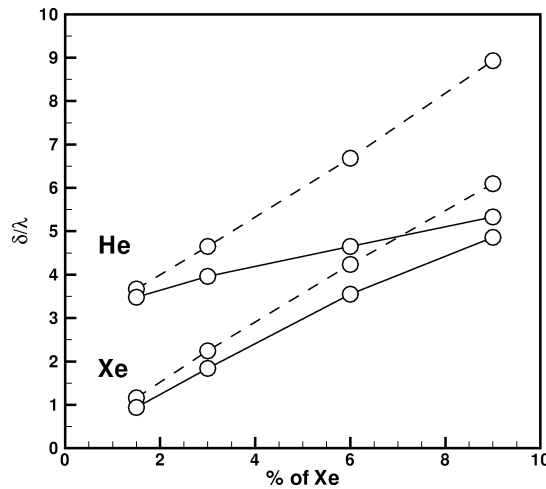


Figure 6. Shock wave thickness of helium and xenon.

Variants V1, V3 and V4 correspond to the conditions of density measurements by Walenta [23]. The comparison of experimental results with those obtained by the present numerical work leads to the same conclusion.

On the basis of the calculations for variants V1 to V4 the shock-wave thicknesses $\delta_{\text{He}}/\lambda_{\text{He}}$ and $\delta_{\text{Xe}}/\lambda_{\text{Xe}}$ have been plotted in *figure 6* against the concentration of Xe in the upstream mixture and compared with the results of [23]. In this case, the shock-wave thickness is calculated as

$$\delta = \frac{\rho_2 - \rho_1}{\max(\partial\rho/\partial x)}. \quad (53)$$

The mean free path for each component is computed according to (48) from the parameters of each gas component ahead of the shock wave. The experimental data are plotted as a solid line; the authors' results as a dashed line. All the curves are represented in the form similar to [23]. For variant V1 (with the smallest Xe concentration), the experimental and computational results coincide practically. For variant V2

the experimental, QGDM and DSMC results are also in good agreement (DSMC shock-wave thickness is not plotted). With increasing Xe concentration, the calculated shock wave thickness is larger than the experimental values. (Note that the He density profiles in the DSMC, QGDM and BGK [17] calculations do not exhibit the overshoot found in the experiment.) Nevertheless, the qualitative behaviour is reproduced by the calculations. This is also consistent with the well-known fact that the relative shock wave thickness increases when the upstream Mach number decreases.

The shock wave thickness is a very sensitive characteristic of the problem, and its calculation based on moment equations for a single-component gas corresponds to the experimental data only in the case of small Mach numbers $Ma \leq 2$.

8. Argon–helium diffusion

As a second example of application of the QGDM equations, the problem of helium and argon mass diffusion was studied for conditions that correspond to a computation by the DSMC method [2]. Let two reservoirs, filled with the gases be located at a distance $L = 1$ m. He is gas a in the right reservoir, and Ar is gas b in the left reservoir. The number densities in the reservoirs are kept constant and equal to $n = 2.8 \cdot 10^{20} \text{ m}^{-3}$. The gases in the reservoirs are assumed to have the same temperature $T = 273$ K and the same velocity equal to zero.

The constants for helium and argon, necessary for the calculations, are shown in *table V* according to [2].

Using these constants, the missing initial data can be obtained: helium density $\rho_a = nm_a = 1.862 \cdot 10^{-6} \text{ kg/m}^3$; sound velocity $a_a = \sqrt{\gamma_a R_a T_a} = 971.9 \text{ m/s}$; mean free path computed by formula (48) $\lambda_a = 1.479 \cdot 10^{-2} \text{ m}$; argon density $\rho_b = nm_b = 1.856 \cdot 10^{-5} \text{ kg/m}^3$; sound velocity $a_b = \sqrt{\gamma_b R_b T_b} = 307.81 \text{ m/s}$; mean free path computed by formula (48) is $\lambda_b = 4.63 \cdot 10^{-3} \text{ m}$.

As in the previous section, computing was performed in dimensionless variables with all quantities normalized by the parameters of gas a – helium in the reservoir. The corresponding non-dimensional parameters are presented in *table VI*.

A one-dimensional plane flow described by equations (42)–(47) was considered. As boundary conditions the following non-dimensional relations were used:
at the left-hand boundary (1)

$$\rho_a = 1. - 10^{-10}, \quad \rho_b = 10^{-10}, \quad T_a = T_b = 1., \quad \frac{\partial u_a}{\partial x} = \frac{\partial u_b}{\partial x} = 0,$$

at the right-hand boundary (2)

$$\rho_b = 1. - 10^{-10}, \quad \rho_a = 10^{-10}, \quad T_a = T_b = 1., \quad \frac{\partial u_a}{\partial x} = \frac{\partial u_b}{\partial x} = 0.$$

That is, we assumed that in each reservoir a fraction $\sim 10^{-10}$ of the other gas exists. At initial time, the density of the components between the reservoirs is assumed to change linearly:

$$\rho_a(x) = \frac{\rho_a(x=L) - \rho_a(x=0)}{L}x + \rho_a(x=0),$$

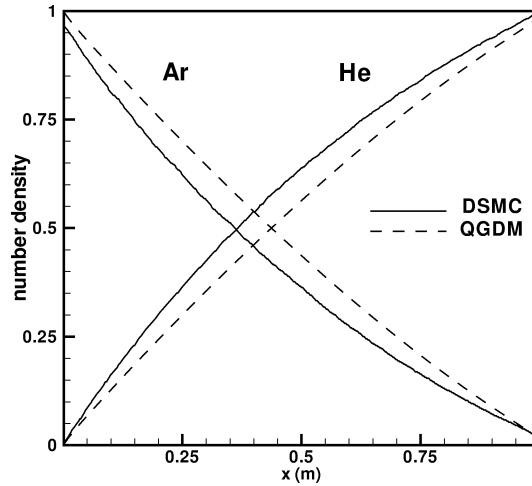
$$\rho_b(x) = \frac{\rho_b(x=L) - \rho_b(x=0)}{L}x + \rho_b(x=0).$$

Table V. Physical properties of mixture components.

	He	Ar
m (kg)	$6.65 \cdot 10^{-27}$	$66.3 \cdot 10^{-27}$
R (J/(kg · K))	2076.2	208.24
\mathcal{M} (kg/mol)	4.0	39.926
d (m)	$2.30 \cdot 10^{-10}$	$4.17 \cdot 10^{-10}$
γ	1.66	1.66
ω	0.66	0.81
Pr	0.666	0.666
μ_{ref} (N/(m · s)) at $T = 273$ K	$1.865 \cdot 10^{-5}$	$2.117 \cdot 10^{-5}$

Table VI. Non-dimensional parameters.

	Gas a (He)	Gas b (Ar)
ρ	1.	9.969
T	1.	1.
a	1.	0.316
λ	1.	0.313
p	0.6	0.60

**Figure 7.** Number densities in the Ar–He diffusion problem.

We used the same numerical algorithm as in the previous section when solving the QGDM equations. The problem was solved using a uniform space grid consisting of 339 points with spatial grid step $h = 0.2$, which corresponded to $0.2\lambda_a$ and $0.64\lambda_b$.

The number densities of both gases are plotted in *figure 7* against the position between the reservoirs. Each of them is reduced by the corresponding reservoir density. The diffusion velocities are plotted in *figure 8*. In both figures the comparison with DSMC results [2] is given. Again the present results agree at least qualitatively with the reference results. The point of equal concentration point is shifted from the middle of the domain to the left, closer to the reservoir containing the heavier gas. The diffusion velocity of helium is larger than that of argon. The diffusion velocity of helium exhibits a minimum in the middle of the computational domain.

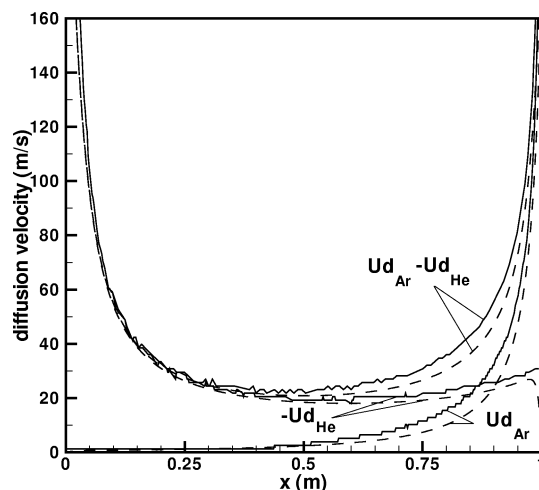


Figure 8. Diffusion velocities in the Ar–He diffusion problem.

9. Conclusion

The macroscopic system of the QGDM equations is constructed on the basis of the kinetic equation system in the relaxation approximation to describe the non-reacting-gas mixture flow. Contrary to some widely known models, the QGDM system consists of the equations for density, momentum and energy of each component, i.e. it is a two-fluid approximation, that makes it possible to describe in detail the behaviour of each component.

The momentum and energy equations include exchange terms, that allow for the appropriate exchanges between the gas components. To calculate these terms the cross-collision frequencies must be estimated. The viscosity of the mixture must also be estimated. The QGDM model includes diffusion processes but does not require coefficients of thermo-, baro- and self- diffusion, which are included in the Navier–Stokes models, and the determination of which is a separate task.

In the present calculations we used quite simple models for the mixture viscosity and for the frequency of cross-collisions and a rather large mass ratio of the species. Nevertheless the QGDM model describes reasonably well the mixture behaviour in the two problems considered. Further improvement can be expected from more accurate expressions.

The system of the QGDM equations is written in an invariant form that allows problems to be solved under various spatial formulations. The algorithms developed on the basis of the QGDM model appear to be more stable than similar algorithms based on the conventional conservation equations.

Thus, the QGDM equations are worth further study for other, future applications.

Acknowledgments

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