Macroscopic equations for a binary gas mixture

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Abstract. The derivation of moment equations for the description of a flowing binary nonreactive gas mixture is presented. The equations obtained are based on a kinetic model in a relaxation form and can be regarded as the extension of the quasigasdynamic equations (QGD) studied before. As an example of implementation the calculations of the shock wave structure for an argon-xenon mixture and of the binary diffusion process for argon and helium, in comparison with the DSMC results are presented.

We consider a mixture consisting of gas a and gas b. Each gas is characterized by its density ρ_i, temperature T_i and macroscopic velocity $\vec{u}_i$, where $i = a, b$. We introduce the gas constant $R_i = k/m_i$, where k is the Boltzmann constant, m_i is the mass of the molecule. According to [1] the kinetical model for the mixture can be expressed as

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

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

where f_a and f_b are the distribution functions for species, $\vec{\xi}$ is the molecule velocity, ν_{aa} and ν_{bb} are the frequencies of self-collisions, ν_{ab} is the frequency of collisions of a molecules with b molecules, ν_{ba} is the frequency of collisions of b molecules with a molecules. F_a, F_b and $\bar{F}_a$, $\bar{F}_b$ are Maxwellian distribution functions based on (u_a, T_a), (u_b, T_b), $(\bar{u}_a, \bar{T}_a)$, $(\bar{u}_b, \bar{T}_b)$. The so-called free parameters (overlined symbols) can be expressed in terms of parameters $m, \vec{u}, T$ of each gas.

We suppose that the distribution functions can be approximated by a gradient expansions as in [2], [3]

$$f_i = F_i - \tau(\vec{\xi}\nabla) F_i \tag{3}$$

where τ is identified with μ/p, μ is the viscosity and p the pressure of the mixture. These expressions are substituted for f_a and f_b into the convective terms of Eqs.1–2 to yield an approximation of these equations

$$\frac{\partial f_a}{\partial t} + (\vec{\xi}\nabla) F_a - (\vec{\xi}\nabla)\tau(\vec{\xi}\nabla) F_a = \nu_{aa}(F_a - f_a) + \nu_{ab}(\bar{F}_a - f_a), \tag{4}$$

$$\frac{\partial f_b}{\partial t} + (\vec{\xi}\nabla) F_b - (\vec{\xi}\nabla)\tau(\vec{\xi}\nabla) F_b = \nu_{bb}(F_b - f_b) + \nu_{ba}(\bar{F}_b - f_b). \tag{5}$$

Equations 4 and 5 are integrated over the velocity space after multiplications by 1, $\vec{\xi}$ and $\vec{\xi}^2/2$, successively and result in a system (QGDM) of macroscopic equations for the binary mixture

$$\frac{\partial}{\partial t}\rho_a + \nabla_i \rho_a\, u_a^i - \nabla_i \tau\,(\nabla_j \rho_a\, u_a^i u_a^j + \nabla^i p_a) = 0, \tag{6}$$

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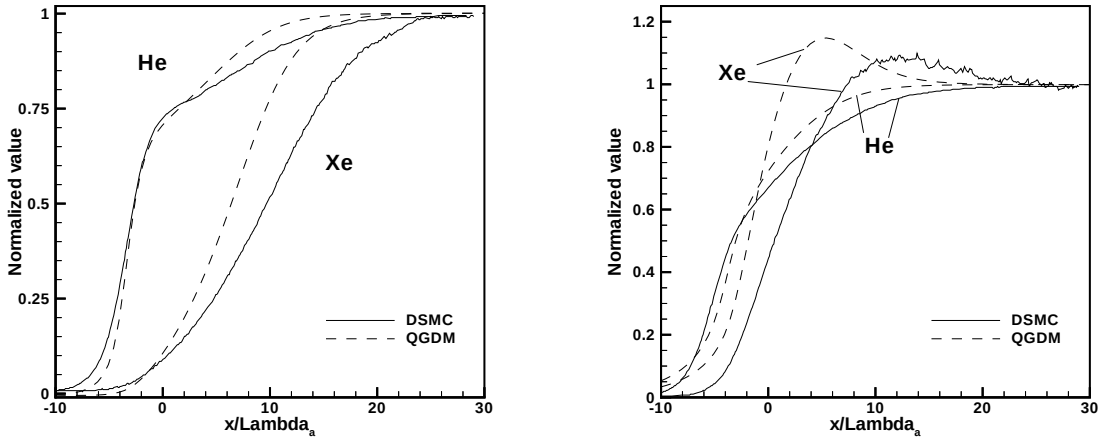

FIGURE 1. Density and temperature profiles in a He-Xe mixture

$$\frac{\partial}{\partial t}\rho_a\, u_a^k + \nabla_i \rho_a\, u_a^i u_a^k + \nabla^k p_a = \nabla_i\, \tau\, (\nabla_j\, \rho_a\, u_a^i u_a^j u_a^k + \nabla^i\, p_a\, u_a^k + \nabla^k\, p_a\, u_a^i) + \nabla^k\, \tau\, \nabla_i\, p_a\, u_a^i + S_a^u, \tag{7}$$

$$\frac{\partial}{\partial t}E_a + \nabla_i u_a^i (E_a + p_a) = \nabla_i\, \tau\, (\nabla_j (E_a + 2p_a)\, u_a^i u_a^j + \frac{1}{2}\nabla^i u_{ak}\, u_a^k p_a) + \frac{\gamma_a}{\gamma_a - 1}\nabla_i\, \tau\, \frac{p_a}{\rho_a}\nabla^i\, p_a + Pr_a^{-1}\frac{\gamma_a}{\gamma_a - 1}\nabla_i\, \tau\, p_a\, \nabla^i \frac{p_a}{\rho_a} + S_a^E, \tag{8}$$

where the volumic energy writes

$$E_a = (\rho_a \vec{u}_a^2)/2 + p_a/(\gamma_a - 1) \qquad \text{with } p_a = \rho_a R_a T_a \tag{9}$$

Similar equations hold for gas b. The Prandtl number Pr and specific heat ratio γ do not appear in the above-described treatment and have been introduced artificially for generalization purpose to make these equations coincide with Navier-Stokes (NS) equations in the case of a one-species gas and vanishing Knudsen numbers ($\tau \to 0$) [4]. The exchange terms S result from the integration of the right-hand sides of the equations and are recognized as

$$S_a^u = \nu_{ab}\rho_a(\bar{\vec{u}}_a - \vec{u}_a), \quad S_b^u = \nu_{ba}\rho_b(\bar{\vec{u}}_b - \vec{u}_b), \quad S_a^E = \nu_{ab}(\bar{E}_a - E_a), \quad S_b^E = \nu_{ba}(\bar{E}_b - E_b), \tag{10}$$

where $\bar{E}_a$ and $\bar{E}_b$ have expressions similar to E_a in Eq.9. ν_{ab} is taken from equilibrium gas formulas and ν_{ba} results from the balance $n_a\, \nu_{ab} = n_b\, \nu_{ba}$. Thus the binary mixture has been described by a self-contained set of two-fluid equations which allow for different velocities and temperatures for the components.

As a first example of application, we considered the structure of a shock wave in a He-Xe mixture under conditions that have been investigated experimentally. Only those variants which have also been calculted by DSMC [5] are reported here in Fig.1. Upstream Mach numbers were 2.78 for He and 15.93 for Xe. Concentrations were 97% for He and 3% for Xe. QGDM results appear to be in reasonable agreement with DSMC results. Results for other flow parameters will be presented as the diffusion of a He-Ar mixture.

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