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Heat transfer in gas mixtures: Advantages of an extended thermodynamics approach

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ABSTRACT

In this work we analyze and compare different approaches to the heat transfer problem in gas mixtures. Our aim is to show that for rarefied gases far from equilibrium the extended thermodynamics description is capable to reproduce some features observed by kinetic theory, that cannot be described by the Navier–Stokes–Fourier–Fick approximations. In this framework, we consider the case of a binary inert gas mixture confined between two infinite parallel plates kept at different temperatures.

1. Introduction

Gas mixtures are usually described following two different approaches: through models obtained at a microscopic level by the kinetic theory [1–5] or by means of models derived at a macroscopic level from the continuum theory [6–13]. For simplicity, the macroscopic description of a mixture is often accompanied by the assumption of a common temperature for all the constituents, at least when the atomic masses of the species do not differ too much, and also in the present Letter we will refer to this simplifying hypothesis.

A kinetic description is surely more accurate than continuum phenomenological models, but requires much more computational time to get precise results. For this reason fluid mixtures are often described referring to the Navier–Stokes–Fourier–Fick approximations with a single common temperature (NSFF). Such a model could be satisfactory for dense gases, but it is surely not appropriate for rarefied gases or when strong deviations from equilibrium occur. In these cases, for single fluids, Extended Thermodynamics (ET) provides better results [13]. That's why we shall analyze here a very simple single-temperature ET model that can be also viewed as a Grad equation system [14] for multi-component fluids. We will compare its predictions with those obtained by NSFF equations and by kinetic theory (Boltzmann equation). To this aim, we will refer to steady heat transfer between parallel plates in rarefied gases, since it is one of the simplest non-equilibrium physical examples and represents a first good test run for the validation and comparison of different approaches to the mixture description. What is already known in the literature is that NSFF system fails to take into account one of the most peculiar behavior of a mixture: the thermal diffusion [3,8]. Is an ET single-temperature model able to catch such a phenomenon? In what follows we will try to answer to this question.

2. Field equations

In the framework of rational thermodynamics [6,9], fluid mixtures are treated assuming that for each component it is possible to write the same balance laws as for a single fluid (except for the production terms). Furthermore, the equations for the entire mixture are the same as for a single fluid. Here, we will follow this theory for both classical and extended thermodynamics. We will focus on a binary inert gas mixture in a stationary regime and refer to the index $\alpha = 1, 2$ for the two constituents, assuming that the two atomic masses satisfy the condition $m_1 < m_2$.

2.1. An extended thermodynamics single-temperature model

The simplest extended thermodynamics model for a homogeneous gas mixture is the single-temperature system proposed by Heckl and Müller [10] and also studied by Kremer [12]. In such a theory the field variables are not only the classical ones, like pressures p^α, velocities v_i^α, and common temperature T, but also the

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heat fluxes q_i^α and the traceless parts of the stress tensors $\rho^\alpha_{\langle ik\rangle}$. For these new variables suitable balance laws are derived. The system of field equations is composed by the equations for the entire mixture and those relative to the first constituent.

If we consider the stationary heat transfer problem between two parallel plates, we can suppose that the fields depend only on the space coordinate x (orthogonal to the plates) and that the velocity of the mixture v_i (mass-center velocity) vanishes. Moreover, we will take into account the BGK productions [15]. We will denote by $J_i^\alpha = \rho^\alpha u_i^\alpha$ the diffusion flux, and by $u_i^\alpha = v_i^\alpha - v_i$ and ρ^α respectively the diffusion velocity and the mass density of the α-constituent.

Besides the mass density, in mixture theory one often refers to particle number density and mass concentration, that respectively read

$$n^\alpha = \frac{\rho^\alpha}{m^\alpha}, \qquad c^\alpha = \frac{\rho^\alpha}{\sum_\alpha \rho^\alpha}. \tag{1}$$

Hence, the equations of model [10] reduce to

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[\hat{p}^1 + \hat{p}^2\right] = 0,\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[2\hat{q}^1 + 2\hat{q}^2 + 5\frac{1-r_m}{r_m}\hat{T}\hat{J}^1\right] = 0,\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[5\left(\hat{p}^1 + r_m\hat{p}^2\right)\hat{T} + 7(1-r_m)T\hat{\rho}^1_{\langle 11\rangle}\right]\\
&\quad = -2r_m\frac{\hat{q}^1+\hat{q}^2}{Kn} + 5\frac{1-r_m}{Kn}\hat{T}\hat{J}^1,
\end{aligned} \tag{2}$$

for the mixture

$$\begin{aligned}
&\frac{\mathrm{d}\hat{J}^1}{\mathrm{d}\hat{x}} = 0,\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[\hat{\rho}^1_{\langle 11\rangle} + \hat{p}^1\right] = -\frac{\hat{J}^1}{Kn},\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[5\hat{p}^1\hat{T} + 7\hat{\rho}^1_{\langle 11\rangle}\hat{T}\right] = -\frac{2r_m\hat{q}^1 + 5\hat{T}\hat{J}^1}{Kn},\\
&\frac{4}{15}\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[2\hat{q}^1 + \frac{5}{r_m}\hat{T}\hat{J}^1\right] = -\frac{\hat{\rho}^1_{\langle 11\rangle}}{Kn},
\end{aligned} \tag{3}$$

for the first component, together with the algebraic relations

$$\begin{aligned}
&\hat{\rho}^1_{\langle 11\rangle} + \hat{\rho}^2_{\langle 11\rangle} = 0,\\
&\hat{\rho}^\alpha_{\langle 22\rangle} = \hat{\rho}^\alpha_{\langle 33\rangle} = -\frac{1}{2}\hat{\rho}^\alpha_{\langle 11\rangle}.
\end{aligned} \tag{4}$$

Eqs. $(2)_{1,2}$ represent the conservation laws of momentum and energy for the whole mixture, while $(3)_{1,2}$ are respectively the conservation law of mass (no chemical reaction is taken into account) and the balance law of momentum for the first constituent. In addition, $(2)_3$ and $(3)_3$ are the balance laws for the heat fluxes relative to the whole mixture and to the first constituent. Finally, $(3)_4$ and (4) represent the balance laws for the stress tensor.

The field equations (2)–(4) are written in terms of the dimensionless fields and parameters

$$\begin{aligned}
&\hat{x} = \frac{x}{L}, \qquad \hat{T} = \frac{T}{T_0}, \qquad \hat{n}^\alpha = \frac{n^\alpha}{n_0^1 + n_0^2},\\
&\hat{q}^\alpha = \frac{q^\alpha}{P\sqrt{k_B T_0/m_2}}, \qquad \hat{p}^\alpha = \frac{p^\alpha}{P}, \qquad \hat{\rho}^\alpha_{\langle ij\rangle} = \frac{\rho^\alpha_{\langle ij\rangle}}{P},\\
&\hat{J}^\alpha = \frac{J^\alpha\sqrt{k_B T_0/m_2}}{P}, \qquad r_m = \frac{m_1}{m_2}, \qquad Kn = \frac{\tau\sqrt{k_B T_0/m_2}}{L},
\end{aligned} \tag{5}$$

where L is the gap between the plates, T_0, P and n_0^α suitable values of the common temperature, the total pressure and the number densities, while Kn plays the role of the Knudsen number related to the heaviest component of the mixture as in [4].

The variables that do not appear in system (2)–(4) vanish identically.

2.2. Classical thermodynamics single-temperature approach

The classical approach to inert mixture theory, with a single common temperature and under the same assumptions made for the extended thermodynamics model, introduces the following field equations

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[\hat{p}^1 + \hat{p}^2\right] = 0,\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[2\hat{q}^1 + 2\hat{q}^2 + 5\frac{1-r_m}{r_m}\hat{T}\hat{J}^1\right] = 0,\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[5\left(\hat{p}^1 + r_m\hat{p}^2\right)\hat{T}\right] = -2r_m\frac{\hat{q}^1+\hat{q}^2}{Kn} + 5\frac{1-r_m}{Kn}\hat{T}\hat{J}^1,
\end{aligned} \tag{6}$$

for the mixture

$$\begin{aligned}
&\frac{\mathrm{d}\hat{J}^1}{\mathrm{d}\hat{x}} = 0,\\
&\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left[\hat{\rho}^1_{\langle 11\rangle} + \hat{p}^1\right] = -\frac{\hat{J}^1}{Kn},\\
&5\hat{p}^1\frac{\mathrm{d}\hat{T}}{\mathrm{d}\hat{x}} = -2r_m\frac{\hat{q}^1}{Kn},\\
&\frac{4}{3}\hat{p}^1\frac{\mathrm{d}\hat{v}^1}{\mathrm{d}\hat{x}} = -\frac{\hat{\rho}^1_{\langle 11\rangle}}{Kn},
\end{aligned} \tag{7}$$

for the first component, together with the relations (4).

In Eq. $(7)_4$ we introduced the dimensionless velocity $\hat{v}^1 = v^1/\sqrt{k_B T_0/m_2}$. This is related to the dimensionless diffusion flux through the relation $\hat{J}^1 = \hat{\rho}^1\hat{v}^1$, where $\hat{\rho}^1 = r_m\hat{p}^1/\hat{T}$.

Eqs. $(6)_{1,2}$ and $(7)_{1,2}$ coincide with those of the ET theory, while $(6)_3$ and $(7)_3$ represent the Fourier law appropriate to the whole mixture and to the first component. Then, (4) and $(7)_4$ recover the Navier–Stokes law.

In particular, $(7)_2$ is a generalization of the Fick law, that follows from the balance law of momentum for the first mixture constituent.

3. Boundary conditions and calculation

Here we will consider a stationary regime and impermeable walls. So, the diffusion fluxes of the mixture components will vanish at a boundary and, from $(2)_1$, it is deduced that $\hat{J}^1 = 0$, $\forall\hat{x}$. Furthermore, four other conditions can be associated to this problem. First of all, we can impose two boundary conditions prescribing the values of the common temperature at both plates. Moreover, in a real experiment the total amount of each constituent is assigned, so here it is reasonable to fix the values of the average number densities of both species. It can be easily shown that this condition for the previous models is mathematically equivalent to prescribe the total pressure at a wall and the ratio between the average number densities of the two components. Unfortunately, from an analytical and numerical point of view it is very difficult to solve the equation system imposing directly such constraints for the average densities. For this reason, in what follows, we will assign the number density values of both components at the right boundary (n_R^α), choosing them in such a manner that the previous conditions about the total pressure and the ratio of the average densities are