XVIII International Conference on Hyperbolic Problems
Theory, Numerics, Applications
Málaga, June 20-24, 2022

Asymptotic Derivation of Multicomponent Compressible Flows with Heat Conduction and Mass Diffusion

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Multicomponent systems of fluids occur often in nature and in industry: the Earth's atmosphere consists of nitrogen, oxygen, argon, carbon dioxide and small amounts of other gases. Natural gas is made of gaseous hydrocarbons such as methane, ethane, propane. The widespread presence of multicomponent fluids suggests the importance in understanding their modeling and being able to predict their behavior.

In a multicomponent theory with primitive variables mass density, velocity and temperature, one distinguishes among three classes of models: In a Type-I model, each component is described by its own mass density, but the components move with a common velocity and have a common temperature. In Type-II models, each component is described by its own mass density and velocity, but the components have a common temperature. Type-III models (which are not considered here) are described via the individual densities, velocities and temperatures of each component.

To this end, consider the Type-II system of equations for multicomponent fluids:

$$\partial_t \rho_i + \text{div}(\rho_i v_i) = 0 \tag{1}$$

$$\partial_t(\rho_i v_i) + \text{div}(\rho_i v_i \otimes v_i) = \rho_i b_i - \rho_i \nabla \mu_i - \frac{1}{\theta}(\rho_i e_i + p_i - \rho_i \mu_i)\nabla\theta - \frac{\theta}{\epsilon}\sum_{j\neq i} b_{ij}\rho_i\rho_j(u_i - u_j) \tag{2}$$

$$\begin{aligned} &\partial_t\left(\rho e + \sum_i \frac{1}{2}\rho_i v_i^2\right) + \text{div}\left(\left(\rho e + \sum_i \frac{1}{2}\rho_i v_i^2\right) v\right) \\ &= \text{div}\left(\kappa\nabla\theta - \sum_i(\rho_i e_i + p_i + \frac{1}{2}\rho_i v_i^2)u_i\right) - \text{div}(pv) + \rho b \cdot v + \rho r + \sum_i \rho_i b_i \cdot u_i \end{aligned} \tag{3}$$

Equations (1) are the partial mass balances and (2) the partial momentum balances of the n components of the fluid, while (3) is the balance of total energy of the mixture. The index $i \in \{1, \dots, n\}$ refers to the i-th component of the fluid. The prime variables are the mass densities ρ_i, the partial velocities v_i and the temperature of the mixture θ. We define the total mass $\rho = \sum_i \rho_i$, the barycentric velocity of the mixture $v := \frac{1}{\rho}\sum_i \rho_i v_i$ and the diffusional velocities $u_i := v_i - v$; the latter satisfy $\sum_i \rho_i u_i = 0$. Moreover, we have the following thermodynamic quantities: the chemical potentials μ_i, the partial pressures p_i, the specific internal energies e_i and we define the total pressure $p = \sum_i p_i$ and the thermal energy $\rho e = \sum_i \rho_i e_i$. Furthermore, b_i stands for the body forces acting on the i-th component and r_i for the heat supply due to radiation, where $\rho b = \sum_i \rho_i b_i$ is the total body force and $\rho r = \sum_i \rho_i r_i$ the total heat supply due to radiation. Finally, $\kappa = \kappa(\rho_1, \dots, \rho_n, \theta) \geq 0$ is the heat conductivity and $b_{ij} = b_{ij}(\rho_i, \rho_j, \theta)$ are nonnegative and symmetric coefficients that model the interaction between the i-th and j-th components with a strength that is measured by $\epsilon > 0$.

The system is complemented by a set of constitutive relations, which read

$$\rho\psi = \rho\psi(\rho_1, \dots, \rho_n, \theta) \tag{4}$$

$$\rho\psi = \rho e - \rho\eta\theta \tag{5}$$

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$$(\rho\psi)_{\rho_i} = \mu_i \tag{6}$$

$$(\rho\psi)_\theta = -\rho\eta \tag{7}$$

where $\rho\psi$ is the Helmholtz free-energy and $\rho\eta$ the entropy, along with the Gibbs-Duhem relation, for determining the total pressure:

$$\rho\psi + p = \sum_i \rho_i\mu_i \tag{8}$$

The format of equations (4)-(7) is motivated by the usual considerations of equilibrium thermodynamics, while the model is consistent with the Clausius-Duhem inequality.

In addition to system (1)-(3), consider also the system

$$\partial_t\rho_i + \mathrm{div}(\rho_i v) = -\mathrm{div}(\epsilon\rho_i\tilde{u}_i) \tag{9}$$

$$\partial_t(\rho v) + \mathrm{div}(\rho v\otimes v) = \rho b - \nabla p \tag{10}$$

$$\begin{aligned}\partial_t\left(\rho e + \frac{1}{2}\rho v^2\right) + \mathrm{div}\left((\rho e + \frac{1}{2}\rho v^2)v\right) &= \mathrm{div}\left(\kappa\nabla\theta - \epsilon\sum_i(\rho_i e_i + p_i)\tilde{u}_i\right)\\ &\quad - \mathrm{div}(pv) + \rho r + \rho b\cdot v + \sum_i \rho_i b_i\cdot u_i\end{aligned} \tag{11}$$

where $u_i = \epsilon\tilde{u}_i$ is determined by solving the constrained algebraic system of Maxwell-Stefan type

$$\begin{aligned}-\sum_{j\neq i} b_{ij}\theta\rho_i\rho_j(u_i - u_j) &= \epsilon\left(-\frac{\rho_i}{\rho}\nabla p + \rho_i\theta\nabla\frac{\mu_i}{\theta} - \theta(\rho_i e_i + p_i)\nabla\frac{1}{\theta}\right)\\ \sum_i \rho_i u_i &= 0\end{aligned} \tag{12}$$

The system (9)-(12) forms a Type-I model, with the same notation as before and the same constitutive relations.

The focus of the present work is on the system (9)-(12) modeling non-isothermal multi-component flows that include the effects of mass-diffusion and heat conduction but no viscous effects. As is typical for Maxwell-Stefan systems, a key difficulty arises from the inversion of (12). First, the Chapman-Enskog analysis (which is known for the isothermal case) is extended to the non-isothermal case thus obtaining an asymptotic derivation of the Type-I model from the Type-II model (1)-(3). Next, system (1)-(3) is complemented with its corresponding entropy identity and, by performing an asymptotic analysis to the entropy identity, we obtain the entropy identity for the system (9)-(12). This analysis indicates how the emerging system inherits the dissipative structure of the original system.

The second step is to verify that (9)-(12) fits into the general framework of systems of hyperbolic-parabolic type. There are two aspects to this question: (i) to address the connection between the "mathematical entropy" and the thermodynamic structure of the model and (ii) to identify the dissipative structure of mass-diffusion and heat conduction. The latter connects to the issue of inversion of the constrained algebraic system (12). This is overcome by using the notion of the Bott-Duffin inverse of a matrix, which provides an important ingredient for inverting the algebraic system and comparing the entropic structure of the Type-I model with the usual entropic structure of hyperbolic-parabolic systems.

Third, we derive a relative entropy identity for (9)-(12), which monitors the evolution of the relative entropy and is remarkable in its simplicity. This identity is, in turn, used in order to prove convergence from strong solutions of the system (9)-(12) to strong solutions of heat-conducting multicomponent Euler system when the mass-diffusivity ϵ tends to zero. Also to prove convergence to smooth solutions of multi-component adiabatic Euler flows when both heat conductivity κ and mass diffusivity ϵ tend to zero.