Derivation of Maxwell-Stefan and Fick cross-diffusion models from the multi-species Boltzmann equation in the diffusive scaling

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Outline of the talk

Introduction

- Context of the study
- Gaseous mixtures: macroscopic models
- Kinetic setting

2 Moment method

- 3 Perturbative method
- 4 Stiff dissipative hyperbolic formalism
- 5 Conclusion and prospects

Context of the study

- Non-reactive mixture of p monoatomic gases
- Isothermal setting T > 0 uniform and constant
- Two different scales for the description of the mixture
 - mesoscopic scale (kinetic model): species i described by its distribution function f_i(t, x, v)
 - macroscopic scale: species i described by the physical observables
 - number density $n_i(t, x)$
 - velocity u_i(t, x)

 \rightarrow average velocity of species i: $J_i(t, x) = n_i(t, x)u_i(t, x)$

 \rightsquigarrow vectorial quantities $\mathbf{n} = \begin{vmatrix} n_1 \\ \vdots \\ \vdots \end{vmatrix}$, $\mathbf{J} = \begin{vmatrix} J_1 \\ \vdots \\ \vdots \\ \vdots \end{vmatrix}$

Diffusion models for mixtures: Maxwell-Stefan/Fick

Mass conservation:

 $\partial_t \mathbf{n} + \nabla \cdot \mathbf{J} = \mathbf{0}$

Diffusion process (link between **J** and ∇ **n**):



• $A(\mathbf{n})$ and $B(\mathbf{n})$ are not invertible (rank p-1)

Using Moore-Penrose pseudo-inverse: structural similarity

Formal analogy of the two systems, but Fick and Maxwell-Stefan are not obtained in the same way

Maxwell-Stefan vs. Fick (macroscopic point of view)

Obtention of the Maxwell-Stefan equations

- Mechanical considerations on forces (balance of pressure and friction forces)
- Assumption: different species have different macroscopic velocities on macroscopic time scales
- Stems from momentum equations

Obtention of the Fick equations

- Thermodynamics of irreversible processes (entropy decay) [Onsager]
- Thermodynamical considerations on fluxes, written (close to equilibrium) as linear combinations of potential gradients
 - nonreactive isothermal setting \rightsquigarrow chemical potential gradients
 - ▶ ideal gases ~→ (number) density gradients
- Stems from mass equations

Maxwell-Stefan vs. Fick (mesoscopic point of view)

Two main questions

- How to justify these two (different) equations from the (same) kinetic description?
- Is there a link between the Maxwell-Stefan and the Fick diffusion coefficients?
- In which regime are these macroscopic models valid?

Moment method (Maxwell-Stefan)

 Based on the ansatz that the distribution functions are at local Maxwellian states [Levermore], [Müller, Ruggieri]

Perturbative method (Fick)

 Based on the Chapman-Enskog expansion [Bardos, Golse, Levermore], [Bisi, Desvillettes]

Kinetic setting

• Elastic collision rules, for $\sigma \in \mathbb{S}^{d-1}$

$$\begin{cases} v' = (m_i v + m_k v_* + m_k | v - v_* | \sigma) / (m_i + m_k), \\ v'_* = (m_i v + m_k v_* - m_i | v - v_* | \sigma) / (m_i + m_k) \end{cases}$$

• Boltzmann collision operator, for $v \in \mathbb{R}^d$

$$Q_{ij}(f_i,f_j)(\mathbf{v}) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \mathcal{B}_{ij}(\mathbf{v},\mathbf{v}_*,\sigma) \Big[f_i(\mathbf{v}') f_j(\mathbf{v}'_*) - f_i(\mathbf{v}) f_j(\mathbf{v}_*) \Big] \mathrm{d}\sigma \mathrm{d}\mathbf{v}_*$$

- Cross sections $\mathcal{B}_{ij} = \mathcal{B}_{ji} > 0$
- Boltzmann equations for mixtures

$$\partial_t f_i + \mathbf{v} \cdot \nabla_x f_i = \sum_{j=1}^p Q_{ij}(f_i, f_j), \quad \text{on } \mathbb{R}_+ \times \Omega \times \mathbb{R}^d, \quad 1 \leq i \leq p$$

[Desvillettes, Monaco, Salvarani, '05]

Properties of the collision operator

Equilibrium: Maxwellian with same bulk velocity and temperature

$$n_i(t,x)\left(\frac{m_i}{2\pi k_BT}\right)^{d/2} \exp\left(-\frac{m_i|v-u(t,x)|^2}{2k_BT}\right)$$

▶ Conservation properties of the collision operator for $1 \le i, j \le p$.

$$\begin{split} &\int_{\mathbb{R}^d} Q_{ij}(f_i,f_j)(v) \,\mathrm{d}v = 0, \qquad \int_{\mathbb{R}^d} Q_{ii}(f_i,f_i)(v)v \,\mathrm{d}v = 0, \\ &\int_{\mathbb{R}^d} \left(m_i Q_{ij}(f_i,f_j)(v) + m_j Q_{ji}(f_j,f_i)(v) \right) \frac{v^2}{2} \,\mathrm{d}v = 0 \end{split}$$

Diffusive scaling

Small mean free path and Mach number: Kn \sim Ma $\sim arepsilon$

$$\varepsilon \partial_t f_i^{\varepsilon} + v \cdot \nabla_x f_i^{\varepsilon} = rac{1}{\varepsilon} \sum_{j=1}^p Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon}), \qquad 1 \le i \le p$$

Properties of the collision operator & Diffusive scaling

Equilibrium: Maxwellian with same bulk velocity and temperature

$$n_i(t,x)\left(\frac{m_i}{2\pi k_BT}\right)^{d/2} \exp\left(-\frac{m_i|v-u(t,x)|^2}{2k_BT}\right)$$

• Conservation properties of the collision operator for $1 \le i, j \le p$.

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Diffusive scaling

Small mean free path and Mach number: ${\rm Kn} \sim {\rm Ma} \sim \varepsilon$

$$\varepsilon \partial_t f_i^{\varepsilon} + v \cdot \nabla_x f_i^{\varepsilon} = \frac{1}{\varepsilon} \sum_{j=1}^p Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon}), \qquad 1 \le i \le p$$

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Moment method

Moments of the distribution functions

Number density of species i

$$n_i^{\varepsilon}(t,x) = \int_{\mathbb{R}^d} f_i^{\varepsilon}(t,x,v) \mathrm{d}v$$

Flux of species i

$$J_i^{\varepsilon}(t,x) = n_i^{\varepsilon}(t,x) \, u_i^{\varepsilon}(t,x) = \frac{1}{\varepsilon} \int_{\mathbb{R}^d} v \, f_i^{\varepsilon}(t,x,v) \mathrm{d}v$$

Ansatz

The distribution function of each species *i* is at a local Maxwellian state with a small velocity of order ε for any $(t, x) \in \mathbb{R}_+ \times \Omega$

$$f_i^{\varepsilon}(t, x, v) = n_i^{\varepsilon}(t, x) \left(\frac{m_i}{2\pi k_B T}\right)^{d/2} \exp\left(-\frac{m_i |v - \varepsilon u_i^{\varepsilon}(t, x)|^2}{2k_B T}\right)$$

Macroscopic diffusion equations

$$\varepsilon \partial_t f_i^{\varepsilon} + \mathbf{v} \cdot \nabla_x f_i^{\varepsilon} = rac{1}{arepsilon} \sum_j Q_{ij}(f_i^{arepsilon}, f_j^{arepsilon}), \quad \forall i \in \llbracket 1, p
rbracket$$

Mass conservation: moment of order 0 $\varepsilon \frac{\partial}{\partial r} \left(\int f_i^{\varepsilon}(\mathbf{v}) d\mathbf{v} \right) + \nabla_{\mathbf{v}} \cdot \left(\int \mathbf{v} f_i^{\varepsilon}(\mathbf{v}) d\mathbf{v} \right) = 0$

$$= \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^3} f_i^{\varepsilon}(\mathbf{v}) \, \mathrm{d}\mathbf{v} \right) + \nabla_{\mathbf{x}} \cdot \left(\int_{\mathbb{R}^3} \mathbf{v} \, f_i^{\varepsilon}(\mathbf{v}) \, \mathrm{d}\mathbf{v} \right) = 0,$$

where the collision term vanishes (conservation property).

Momentum equation: moment of order 1 $\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^3} v f_i^{\varepsilon}(v) dv + \int_{\mathbb{R}^3} v (v \cdot \nabla_x f_i^{\varepsilon}(v)) dv = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^3} v Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon})(v) dv$

where the mono-species collision term vanishes (conservation property).

Computation of the divergence term

$$\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^3} v f_i^{\varepsilon}(v) \, dv + \left| \int_{\mathbb{R}^3} v \left(v \cdot \nabla_x f_i^{\varepsilon}(v) \right) \, dv \right| = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^3} v \, Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon})(v) \, dv$$

• Use of the Ansatz, translation in v + parity argument

$$\nabla_{\mathbf{x}} \cdot \left(\int \mathbf{v} \otimes \mathbf{v} \, f_i^{\varepsilon}(\mathbf{v}) \, \mathrm{d}\mathbf{v}\right) \propto \nabla_{\mathbf{x}} \cdot \left(n_i^{\varepsilon} \int \left(\mathbf{v} \otimes \mathbf{v} + \varepsilon^2 u_i^{\varepsilon} \otimes u_i^{\varepsilon}\right) e^{-m_i |\mathbf{v}|^2/2kT} \mathrm{d}\mathbf{v}\right)$$

In terms of macroscopic quantities

$$\nabla_{\mathsf{x}} \cdot \left(\int \mathsf{v} \otimes \mathsf{v} \, f_i^{\varepsilon}(\mathsf{v}) \, \mathrm{d} \mathsf{v} \right) = \frac{k_B T}{m_i} \nabla_{\mathsf{x}} n_i^{\varepsilon} + \varepsilon^2 \nabla_{\mathsf{x}} \cdot \left(n_i^{\varepsilon} \, u_i^{\varepsilon} \otimes u_i^{\varepsilon} \right)$$

Computation of the collision term

For Maxwell molecules: weak form, collision rules, symmetry and parity arguments:

$$\int v Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon})(\mathbf{v}) \, \mathrm{d}\mathbf{v} = \frac{m_j}{m_i + m_j} \int b_{ij}(\cos \theta) \, f_i^{\varepsilon} f_{j*}^{\varepsilon} \left(\mathbf{v}_* - \mathbf{v} + |\mathbf{v} - \mathbf{v}_*|\sigma\right) \, \mathrm{d}\sigma \, \mathrm{d}\mathbf{v}_* \, \mathrm{d}\mathbf{v}$$

In terms of macroscopic quantities

$$\frac{1}{\varepsilon} \sum_{j \neq i} \int v \, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v) \, \mathrm{d}v = \sum_{j \neq i} \underbrace{\frac{2\pi m_i m_j \|b_{ij}\|_{L^1}}{(m_i + m_j)k_B T}}_{D_{ij}^{-1}} \frac{k_B T}{m_i} \left(n_i^\varepsilon n_j^\varepsilon u_j^\varepsilon - n_j^\varepsilon n_i^\varepsilon u_i^\varepsilon \right)$$

▶ For general cross sections: algebraic arguments [BOUDIN, G., PAVAN, '17]

$$D_{ij} \propto \iiint B_{ij}(\mathbf{v}, \mathbf{v}_*, \sigma) \exp\left[-rac{m_i}{2k_BT}\mathbf{v}^2 - rac{m_j}{2k_BT}\mathbf{v}_*^2
ight](\mathbf{v}'-\mathbf{v})^2$$

Formal asymptotics and limit equation

Formal limit

$$n_i(t,x) = \lim_{\varepsilon \to 0} n_i^{\varepsilon}(t,x), \qquad J_i(t,x) = \lim_{\varepsilon \to 0} n_i^{\varepsilon}(t,x) u_i^{\varepsilon}(t,x)$$

• Mass conservation (order ε^1)

$$\partial_t n_i + \nabla_x \cdot J_i = 0$$

• Momentum equation (order ε^0)

$$\varepsilon^{2} \frac{m_{i}}{k_{B}T} \Big(\partial_{t} (n_{i}^{\varepsilon} u_{i}^{\varepsilon}) + \nabla_{x} \cdot (n_{i}^{\varepsilon} u_{i}^{\varepsilon} \otimes u_{i}^{\varepsilon}) \Big) + \nabla_{x} n_{i}^{\varepsilon} = \sum_{j \neq i} \frac{n_{i}^{\varepsilon} n_{j}^{\varepsilon} u_{j}^{\varepsilon} - n_{j}^{\varepsilon} n_{i}^{\varepsilon} u_{i}^{\varepsilon}}{D_{ij}} + o(1)$$

$$-\nabla_{\mathbf{x}} n_i = \sum_{j \neq i} \frac{n_j J_i - n_i J_j}{D_{ij}}, \qquad i.e. \qquad -\nabla_{\mathbf{x}} \mathbf{n} = A(\mathbf{n}) \mathbf{J}.$$

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Perturbative method

$$\varepsilon \partial_t f_i^{\varepsilon} + \mathbf{v} \cdot \nabla_x f_i^{\varepsilon} = \frac{1}{\varepsilon} \sum_j Q_{ij}(f_i^{\varepsilon}, f_j^{\varepsilon}), \quad \forall i \in [\![1, p]\!]$$

Expansion around the global Maxwellian with zero bulk velocity (equilibrium) with number density n_i

$$\mu_i = n_i \mu_i + \varepsilon g_i^{\varepsilon} \qquad \qquad \mu_i = (m_i/2\pi k_B T)^{d/2} e^{-m_i |\mathbf{v}|^2/2k_B}$$

Moments of the distribution function

 f_i^{ε}

$$J_i(t,x) = \int v f_i^{\varepsilon}(t,x,v) \mathrm{d}v = \int v g_i^{\varepsilon}(t,x,v) \mathrm{d}v$$

Mass conservation: zero-th moment in velocity, order ε^1

$$\partial_t n_i + \nabla_x \cdot J_i = 0$$

• Inject expansion in the Boltzmann equation, order ε^0

$$\mu_i \mathbf{v} \cdot \nabla_{\mathbf{x}} n_i = \sum_j Q_{ij}(n_i \mu_i, g_j^{\varepsilon}) + Q_{ji}(g_i^{\varepsilon}, n_j \mu_j) =: \mathcal{L}_i(\mathbf{g}^{\varepsilon}),$$

where $\mathbf{g}^{\varepsilon} = (g_i^{\varepsilon})_i \rightsquigarrow$ defines the linearized Boltzmann operator $\mathbf{L} = (\mathcal{L}_i)_i$

$$\mathsf{W} = \mathsf{L}(\mathsf{g}^{arepsilon}) \qquad \mathop{\sim}\limits_{(\star)} \qquad \mathsf{g}^{arepsilon} = \mathsf{L}^{-1}\mathsf{W}$$

lnject this expression for g_i^{ε} in the definition of J_i

$$J_i = \int v[\mathbf{L}^{-1}\mathbf{W}]_i \mathrm{d}v = \int n_i \mu_i v[\mathbf{L}^{-1}\mathbf{W}]_i (n_i \mu_i)^{-1} \mathrm{d}v$$

► With
$$\mathbf{C}_i = (\mu_j v \delta_{ij})_j$$
, we get
$$J_i = n_i \langle \mathbf{C}, \mathbf{L}^{-1} \mathbf{W} \rangle_{L^2((n\mu)^{-1/2})}$$

► L⁻¹ is self-adjoint on $(\text{Ker } \mathbf{L})^{\perp}$. Let $\mathbf{\Gamma}$ be the projection of \mathbf{C} on $\text{Ker } \mathbf{L}$. Thus $J_{i} = n_{i} \sum_{j} \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_{j}, W_{j} \rangle_{L^{2}((n\mu)^{-1/2})}$ ► Since $W_{j} = \mu_{j} \mathbf{v} \cdot \nabla_{\mathbf{x}} n_{j} = \text{``C}_{j} \cdot \nabla_{\mathbf{x}} n_{j}$ $J_{i} = \sum_{j} \underbrace{n_{i} \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_{j}, \mathbf{C}_{j} \rangle_{L^{2}((n\mu)^{-1/2})}}_{b_{ij}(n_{i})} \nabla_{\mathbf{x}} n_{j}$

$$\mathsf{W} = \mathsf{L}(\mathsf{g}^{arepsilon}) \qquad \stackrel{\leadsto}{\underset{(\star)}{\longrightarrow}} \qquad \mathsf{g}^{arepsilon} = \mathsf{L}^{-1}\mathsf{W}$$

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$$J_i = n_i \langle \mathbf{C}, \mathbf{L}^{-1} \mathbf{W} \rangle_{L^2((n\mu)^{-1/2})}$$

▶ L^{-1} is self-adjoint on $(Ker L)^{\perp}$. Let Γ be the projection of C on Ker L. Thus $J_i = n_i \sum_i \langle [\mathbf{L}^{-1} (\mathbf{C} - \mathbf{\Gamma})]_j, W_j \rangle_{L^2((n\mu)^{-1/2})}$ ► Since $W_i = \mu_i v \cdot \nabla_x n_i = "\mathbf{C}_i \cdot \nabla_x n_i"$ $J_i = \sum_i \underbrace{n_i \langle [\mathbf{L}^{-1} (\mathbf{C} - \mathbf{\Gamma})]_j, \mathbf{C}_j \rangle_{L^2((n\mu)^{-1/2})}}_{X_x n_j} \nabla_x n_j$

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$$\mathsf{W} = \mathsf{L}(\mathsf{g}^{arepsilon}) \qquad \stackrel{\leadsto}{\underset{(\star)}{\longrightarrow}} \qquad \mathsf{g}^{arepsilon} = \mathsf{L}^{-1}\mathsf{W}$$

► Inject this expression for g^ε_i in the definition of J_i

$$J_i = \int v[\mathbf{L}^{-1}\mathbf{W}]_i \mathrm{d}v = \int \underline{n_i \mu_i} v[\mathbf{L}^{-1}\mathbf{W}]_i (\underline{n_i \mu_i})^{-1} \mathrm{d}v$$

► With
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► **L**⁻¹ is self-adjoint on (Ker **L**)[⊥]. Let **Γ** be the projection of **C** on Ker **L**. Thus $J_{i} = n_{i} \sum_{j} \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_{j}, W_{j} \rangle_{L^{2}((n\mu)^{-1/2})}$ ► Since $W_{j} = \mu_{j} \mathbf{v} \cdot \nabla_{\mathbf{x}} n_{j} = \text{``C}_{j} \cdot \nabla_{\mathbf{x}} n_{j}$ '' $J_{i} = \sum_{j} \underbrace{n_{i} \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_{j}, \mathbf{C}_{j} \rangle_{L^{2}((n\mu)^{-1/2})}}_{b_{j}(n_{i})} \nabla_{\mathbf{x}} n_{j}$

$$\mathsf{W} = \mathsf{L}(\mathsf{g}^{arepsilon}) \qquad \stackrel{\leadsto}{\underset{(\star)}{\longrightarrow}} \qquad \mathsf{g}^{arepsilon} = \mathsf{L}^{-1}\mathsf{W}$$

► Inject this expression for g^ε_i in the definition of J_i

$$J_i = \int v[\mathbf{L}^{-1}\mathbf{W}]_i \mathrm{d}v = \int \underline{n_i \mu_i v}[\mathbf{L}^{-1}\mathbf{W}]_i (\underline{n_i \mu_i})^{-1} \mathrm{d}v$$

► With
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► \mathbf{L}^{-1} is self-adjoint on $(\text{Ker } \mathbf{L})^{\perp}$. Let $\mathbf{\Gamma}$ be the projection of \mathbf{C} on Ker \mathbf{L} . Thus $J_{i} = n_{i} \sum_{j} \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_{j}, W_{j} \rangle_{L^{2}((n\mu)^{-1/2})}$ ► Since $W_{j} = \mu_{j} \mathbf{v} \cdot \nabla_{\mathbf{x}} n_{j} = \text{``C}_{j} \cdot \nabla_{\mathbf{x}} n_{j}$ $J_{i} = \sum_{j} \underbrace{n_{i} \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_{j}, \mathbf{C}_{j} \rangle_{L^{2}((n\mu)^{-1/2})}}_{b_{ij}(n_{i})} \nabla_{\mathbf{x}} n_{j}$

Closure relation (1)

Maxwell-Stefan equation $-\nabla \mathbf{n} = A(\mathbf{n})\mathbf{J}$

- ▶ Summing over *i* the equations (*A* has rank p 1) implies that $\nabla_x \sum_i n_i = 0$
- Ansatz (local Maxwellian) implies

$$\int m_i |v|^2 f_i^{\varepsilon} \mathrm{d}v = 3k_B T n_i^{\varepsilon} + o(\varepsilon), \qquad \int m_i |v|^2 v f_i^{\varepsilon} \mathrm{d}v = 5\varepsilon k_B T J_i^{\varepsilon} + o(\varepsilon).$$

• Moment of order 2 (order ε^1), summing over *i*, and taking the limit $\varepsilon \to 0$

$$3\partial_t \sum_i n_i + 5\nabla_x \cdot \sum_i J_i = 0,$$

where the collision operator disappears by symmetry when summing over *i*.

Combining with mass conservation implies

$$\partial_t \sum_i n_i = \nabla_{\mathsf{x}} \cdot \sum_i J_i = 0$$

Constant total number of molecules ∑_i n_i
 Compatible with equimolar diffusion ∑_i J_i(t, x) = 0

Closure relation (2)

Fick equation $\mathbf{J} = -B(\mathbf{n})\nabla\mathbf{n}$

- Summing over *i* the equations (*B* has rank p-1) implies that $\sum_{i} m_i J_i = 0$
- ▶ Inversion giving the perturbation \mathbf{g}^{ε} (relation (*)) only valid if the RHS $W_i = \mu_i \mathbf{v} \cdot \nabla_{\mathbf{x}} n_i \in (\text{Ker } \mathbf{L})^{\perp}$.
- Ker L spanned by $(\sqrt{n_i}\mu_i\mathbf{e}_i)_i$, $m_in_i\mu_iv$, $m_in_i\mu_i|v|^2$
- Orthogonality

$$0 = \sum_{i} \int \mu_{i} \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{n}_{i} \mathbf{m}_{i} \mathbf{v} \mathrm{d} \mathbf{v} = \nabla_{\mathbf{x}} \sum_{i} \mathbf{m}_{i} \mathbf{n}_{i}$$

• Mass conservation for each species implies (when summing with weights m_i)

$$0=\frac{\mathrm{d}}{\mathrm{dt}}\int\sum_{i}m_{i}n_{i}\mathrm{d}x$$

• Constant mass $\sum_i m_i n_i$

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Stiff dissipative model for mixtures

For any species *i* with mass density ρ_i and velocity \boldsymbol{u}_i , we write mass and momentum conservation

$$(*) \begin{cases} \partial_t \rho_i + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i) = 0, \\ \partial_t (\rho_i \mathbf{u}_i) + \nabla_{\mathbf{x}} \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + P_i(\rho_i)) + \frac{1}{\varepsilon} R_i = 0 \end{cases}$$

• Ideal gas law for the partial pressure $P_i(\rho_i) = \rho_i k_B T/m_i$

Relaxation term: friction force exerted by the mixture on species i

$$R_i = \sum_{j \neq i} a_{ij} \rho_i \rho_j (\boldsymbol{u}_j - \boldsymbol{u}_i) = \sum_j \alpha_{ij} \boldsymbol{u}_j$$

Using the formalism of Chen, Levermore, Liu, CPAM, '94

Obtain a reduced system when ε remains small

▶ Derive an approximation of the local equilibrium and its first-order correction

- Build a relevant entropy which ensures...
- ... the hyperbolicity of the local equilibrium approximation...
- ... and the dissipativity of its first-order correction

Steps of the computations

- Internal energy $E_i''(\rho_i) = P_i'(\rho_i)/\rho_i$
- (Strictly convex) entropy $\eta = \sum_{j=1}^{p} \frac{1}{2} \rho_j \boldsymbol{u}_j^2 + E_j(\rho_j)$
- (p+d) independent conserved quantities : $\left[\rho_1, \cdots, \rho_p, \sum_{j=1}^p \rho_j \boldsymbol{u}_j\right]$
- Equilibrium: $[\rho_1, \cdots, \rho_p, \rho_1 \boldsymbol{u}, \cdots, \rho_p \boldsymbol{u}]$ for some \boldsymbol{u}

Formal expansion around the equilibrium & linearization

 \rightsquigarrow expression of the correction provided (pseudo-)inversion of "the gradient of the relaxation term", involving the "flux terms"

$$\sum_{j=1}^{p} \alpha_{ij} \frac{X_j}{\rho_j} = \nabla_{\mathsf{x}} P_i(\rho_i) - \frac{\rho_i}{\rho} \nabla_{\mathsf{x}} P_i(\rho_i)$$

with $\rho = \sum_{i} \rho_{i}$, $P = \sum_{i} P_{i}$

 \rightsquigarrow equation on the conserved quantities with the correction term

Steps of the computations

- Internal energy $E_i''(\rho_i) = P_i'(\rho_i)/\rho_i$
- (Strictly convex) entropy $\eta = \sum_{j=1}^{p} \frac{1}{2} \rho_j u_j^2 + E_j(\rho_j)$
- (p+d) independent conserved quantities : $\left[\rho_1, \cdots, \rho_p, \sum_{j=1}^p \rho_j \boldsymbol{u}_j\right]$
- Equilibrium: $[\rho_1, \cdots, \rho_p, \rho_1 \boldsymbol{u}, \cdots, \rho_p \boldsymbol{u}]$ for some \boldsymbol{u}

Formal expansion around the equilibrium & linearization

 \rightsquigarrow expression of the correction provided (pseudo-)inversion of "the gradient of the relaxation term", involving the "flux terms"

$$X_{i} = \sum_{j=1}^{p} \frac{\beta_{ij}}{\rho_{j}} \left(\nabla_{x} P_{j}(\rho_{j}) - \frac{\rho_{j}}{\rho} \nabla_{x} P \right)$$

with $\rho = \sum_{i} \rho_{i}$, $P = \sum_{i} P_{i}$

 \rightsquigarrow equation on the conserved quantities with the correction term

Maxwell-Stefan vs. Fick

Reduced system involving the bulk velocity $oldsymbol{u}$ for small arepsilon

Let $\rho = \sum_{i} \rho_{i}$, and **u** the mass-weighted averaged (aligned) velocity. System (*) formally reduces to

$$\begin{cases} \partial_t \rho_i + \nabla_{\mathbf{x}} \cdot \left(\rho_i \mathbf{u} - \varepsilon \sum_{j=1}^p \beta_{ij} \frac{\nabla_{\mathbf{x}} P_j}{\rho_j} \right) = \mathbf{0}, \\ \partial_t (\rho \mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} P = \mathbf{0}. \end{cases}$$

where $P = \sum_{j} P_j(\rho_j)$ is the total pressure, and (β_{ij}) are positive constants.

Diffusion correction term of Fick's type (on the mass equation)

• Ideal gases
$$\rightsquigarrow
abla_x P_j \propto
abla
ho_j$$

- Fick equations model mass diffusion in a continuous regime
- ▶ No viscosity term on the momentum equation (convective ≫ diffusive fluxes)
- Maxwell-Stefan equations needed in a moderately rarefied regime

Justification of the Ansatz for the Maxwell-Stefan equations

In a moderately rarefied regime (not so dominant collision process)

- Significant deviation from local equilibrium described by the moment method
- Moment method: approach to compute Galerkin solutions to the Boltzmann equation

[Levermore, JSP '96]

• First finite dimensional subspace $\mathbb{M}_0 = \operatorname{Ker} Q$ spanned by e_1, \dots, e_p , $[m_1v, \dots, m_pv]$ and $[m_1v^2, \dots, m_pv^2]$

 \rightsquigarrow equilibrium with one bulk velocity

Second finite dimensional subspace $\mathbb{M}_1 \supset \mathbb{M}_0$ spanned by e_1, \dots, e_p , $m_1 v e_1, \dots, m_p v e_p$ and $[m_1 v^2, \dots, m_p v^2]$

 \rightsquigarrow local Maxwellian with different macroscopic velocities

Outline of the talk

Introductio

- Context of the study
- Gaseous mixtures: macroscopic models
- Kinetic setting

2 Moment method

- 3 Perturbative method
- 4 Stiff dissipative hyperbolic formalism
- 5 Conclusion and prospects

Conclusion and prospects

Conclusions

- Maxwell-Stefan and Fick equations are obtained formally from the Boltzmann equation for mixtures in the diffusive regime
- Not the same assumption on the macroscopic velocities
- Maxwell-Stefan can describe a moderate rarefied regime

Prospects

- Compare the experimental and theoretical relaxation times
- Taking into account non isothermal effects

Thank you for your attention!



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Maxwell-Stefan and Fick models from the kinetic modelling