A Fick relaxation BGK model for a mixture of polyatomic gases

GUILLON Kévin

Collaboration with Stéphane BRULL and Philippe THIEULLEN

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Introduction - Motivations

$$\mathcal{Q}(f,f) \sim \mathcal{R}(f) = \nu(f)(G(f) - f),$$

- Aim : Construct a BGK operator for a **polyatomic mixture** providing **correct phenomenological coefficients** at hydrodynamic limit (Fick, viscosities)
  - [Giovangigli, 1999] : general derivation,
  - [Brull, Pavan, Schneider (2012)] : monoatomic mixture,
  - [Schneider (2015)] : polyatomic mixture w/ discrete energy.
- In this article, polyatomic mixture w/ continuous energy (formalism derived from [Borgnakke, Larsen (1975)],
- Issues :
  1. Fitting constraints with conservation laws, H theorem, successful entropy minimization [Junk (1999)], correct coefficients,
  2. Performing **inclusive** polyatomic model, **containing monoatomic case**

Contents

Polyatomic gases modelization

- $N \geq 1$ gases, $x, v \in \mathbb{R}^3$, $t \geq 0$, $f(t,x,v,I) = (f_i(t,x,v,I_i))_{1 \leq i \leq N}$,
- $\delta_i \geq 0$, $\delta := \sum_i \frac{n_i}{n} \delta_i$,
- $I_i^{\frac{2}{\delta_i}} \geq 0$ continuous level of internal energy of i, $I =^T (I_1, \ldots, I_N)$,
- Natural inner product, for $g(v,I) = (g_i)_{1 \leq i \leq N}$, $h(v,I) = (h_i)_{1 \leq i \leq N}$:

$$\langle g, h \rangle := \sum_{i=1}^{N} \iint g_i(v, I_i) h_i(v, I_i) dv dI_i$$

- Weighted inner product with a Maxwellian vector $\mathcal{M}$:

$$\langle g, h \rangle_{\mathcal{M}} := \sum_{i=1}^{N} \iint g_i(v, I_i) h_i(v, I_i) \mathcal{M}_i(v, I_i) dv dI_i$$

Macroscopic quantities

$e_i =^T (0, \ldots, 0, \underset{\underset{i}{\uparrow}}{1}, 0, \ldots, 0)$, $\overline{w} = \sum_i w_i e_i$.

- $n_i := \langle f, e_i \rangle$,
- $\rho_i := m_i n_i$,
- $u_i := \frac{1}{m_i} \langle f, v e_i \rangle$,
- $n := \sum_i n_i$, $\rho := \sum_i \rho_i$, $u := \sum_i \frac{\rho_i}{\rho} u_i$,
- $nE_{tr} := \left\langle f, \frac{1}{2}\overline{m}(v-u)^2 \right\rangle = \frac{1}{2} \sum_i \iint m_i (v-u)^2 f_i dv dI_i =: \frac{3}{2} nkT_{tr}$,
- $nE_{int} := \left\langle f, \overline{I^{\frac{2}{\delta}}} \right\rangle = \sum_i \iint I_i^{\frac{2}{\delta_i}} f_i dv dI_i =: \frac{\delta}{2} nkT_{int}$,
- $\mathcal{E} := E_{int} + E_{tr} = \frac{\delta}{2} kT_{int} + \frac{3}{2} kT_{tr} =: \frac{\delta + 3}{2} kT$.

Conservation vectors

Conservation space

The collisional invariants are :

$$
\begin{cases}
\phi_1 = \begin{pmatrix} 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, \phi_N = \begin{pmatrix} 0 \\ \vdots \\ 1 \end{pmatrix} \text{(Mass)} \\
1 \leq j \leq 3, \phi_{N+j} = \begin{pmatrix} m_1 v_{x_j} \\ \vdots \\ m_N v_{x_j} \end{pmatrix} \text{(Total Momentum)} \\
\phi_{N+4} = \begin{pmatrix} \frac{1}{2} m_1 v^2 + I_1^{\frac{2}{\delta_1}} \\ \vdots \\ \frac{1}{2} m_N v^2 + I_N^{\frac{2}{\delta_N}} \end{pmatrix} \text{(Total Energy)}
\end{cases}
$$

$\mathbb{K} = Span(\phi_i, 1 \leq i \leq N+4)$ is the conservation space.

Basic physical requirements

Hypotheses for $\mathcal{R}$

1. Conservation laws: $\langle \mathcal{R}(f), \phi \rangle = 0 \Leftrightarrow \phi \in \mathbb{K}$,
2. H-Theorem:

$$\partial_t \langle f, \log f - 1 \rangle + \nabla \cdot \langle vf, \log f - 1 \rangle = \langle \mathcal{R}(f), \log f \rangle \leq 0,$$

equality iff $f = \mathcal{M}$, with:

$$\mathcal{M}_i = n_i \left(\frac{m_i}{2\pi kT}\right)^{\frac{3}{2}} \left(\frac{1}{kT}\right)^{\frac{\delta_i}{2}} \Lambda_i^{-1} \exp\left(-\frac{m_i(v-u)^2}{2kT} - \frac{I_i^{\frac{2}{\delta_i}}}{kT}\right),$$

$$\Lambda_i = \int_0^\infty \exp\left(-I_i^{\frac{2}{\delta_i}}\right) dI_i = \frac{\delta_i}{2} \Gamma\left(\frac{\delta_i}{2}\right).$$

3. Properties at order 1: $\mathcal{L} := \mathcal{M}^{-1} D(\mathcal{R}(\mathcal{M} \cdot))$ is continuous, self adjoint, < 0 on $\mathbb{K}^\perp$ with $Ker(\mathcal{L}) = \mathbb{K}$.

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Phenomenologic coefficients

Navier-Stokes equations for a mixture:

$$\begin{cases} \partial_t \rho_i + \nabla \cdot (\rho_i u + J_i) = 0, \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u + p + J_u) = 0, \\ \partial_t(\rho E) + \nabla \cdot ((\rho E + p)u) + \nabla \cdot (J_q + J_u \cdot u) = 0. \end{cases}$$

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Thermodynamic of irreversible processes:

- Mass fluxes : $J_i = \sum_{j=1}^{N} L_{ij} \nabla(-\frac{\mu_j}{kT}) + L_{iq} \nabla(-\frac{1}{kT})$,
- Heat flux : $J_q = \sum_{j=1}^{N} L_{qj} \nabla(-\frac{\mu_j}{kT}) + L_{qq} \nabla(-\frac{1}{kT})$,
- Velocity flux :$J_u = -\eta\sigma(u) - \eta_V \nabla \cdot u Id_3$.

Aim: recovering green coefficients at hydrodynamic limit.

Expression of $\mathcal{L}$

Chapman Enskog expansion at order 1 $\Rightarrow \mathcal{L}_i(g) = \frac{(\partial_t + v\cdot\nabla)\mathcal{M}_i}{\mathcal{M}_i}$;

$$\boxed{\mathcal{L}[\mathcal{R}](g) = kT A : \sigma(u) + B \cdot \nabla(-\frac{1}{kT}) + \sum_{j=1}^{N} \Phi_j \cdot \nabla(-\frac{\mu_j}{kT}) - \alpha \nabla \cdot u}$$

$$\Phi_j := P_{\mathbb{K}^\perp}(C_j),\ C_j =^T (0, \ldots, 0, \underset{\substack{\uparrow \\ j}}{v - u}, 0, \ldots, 0),$$

$$A(V)_i := V_i \otimes V_i - \frac{1}{3} V_i^2,\ V_i = \sqrt{\frac{m_i}{kT}}(v - u)$$

$$B(v)_i := (v-u)(\frac{1}{2} kT V_i^2 + I_i^{\frac{2}{\delta_i}} - \frac{nm_i}{\rho}(\frac{\delta+5}{2})kT),$$

$$\alpha(V,I)_i := (\frac{1}{\delta+3} - \frac{1}{3})V_i^2 + \frac{\delta - \delta_i}{\delta+3} + 2\frac{I_i^{\frac{2}{\delta_i}}}{kT(\delta+3)} = -P_{\mathbb{K}^\perp}(\frac{1}{2}V^2) = \frac{1}{kT} P_{\mathbb{K}^\perp}(\overline{I^{\frac{2}{\delta}}})$$

$$\mu_j = -kT \ln\left(\frac{n_j \Lambda_j^{-1}}{\left(\frac{2\pi kT}{m_j}\right)^{\frac{3}{2}}}\right).$$

Link with the phenomenological coefficients

NS identification $\Rightarrow$ Expressions of the CE Fluxes :

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$$J_i[\mathcal{R}] = \langle \Phi_i, g \rangle_{\mathcal{M}} \quad J_u[\mathcal{R}] = kT \langle A - \alpha I_3, g \rangle_{\mathcal{M}} \quad J_q[\mathcal{R}] = \langle B, g \rangle_{\mathcal{M}}$$

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- $\boxed{L_{ij}[\mathcal{R}] = \frac{1}{3} \left\langle \Phi_i, \mathcal{L}[\mathcal{R}]^{-1} \Phi_j \right\rangle_{\mathcal{M}}}$,
- $L_{iq}[\mathcal{R}] = \frac{1}{3} \left\langle \Phi_i, \mathcal{L}[\mathcal{R}]^{-1}(B) \right\rangle_{\mathcal{M}}$, $L_{qj}[\mathcal{R}] = \frac{1}{3} \left\langle B, \mathcal{L}[\mathcal{R}]^{-1} \Phi_j \right\rangle_{\mathcal{M}}$,
- $L_{qq}[\mathcal{R}] = \frac{1}{3} \left\langle B, \mathcal{L}[\mathcal{R}]^{-1}(B) \right\rangle_{\mathcal{M}}$,
- $\boxed{\eta[\mathcal{R}] = -\frac{1}{6} k^2 T^2 \left\langle A, \mathcal{L}[\mathcal{R}]^{-1}(A) \right\rangle_{\mathcal{M}}}$, $\boxed{\eta_V[\mathcal{R}] = -kT \left\langle \alpha, \mathcal{L}[\mathcal{R}]^{-1}(\alpha) \right\rangle_{\mathcal{M}}}$.

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$\mathbb{C} := Span\{\Phi_i, 1 \leq i \leq N\}$ space of Fick constraints.

Inverse problem:

Find $\mathcal{R}(f)$ well defined satisfying $(L[\mathcal{R}], \eta[\mathcal{R}], \eta_V[\mathcal{R}]) = (L^{emp}, \eta^{emp}, \eta_V^{emp})$.

Remark : **Coefficients depend on $\mathcal{L}[\mathcal{R}]^{-1}$ and not $\mathcal{L}[\mathcal{R}]$!**

Properties of the empirical coefficients

Study of the empirical Fick Matrix

1. $\sum_i m_i J_i = 0 \Rightarrow rank(L^{emp}) \leq N-1$ (actually $=$),
2. L^* defined by $L^*_{ij} := k \dfrac{L_{ij}}{||C_i||||C_j||}$ is symmetric (**Casimir-Onsager relations**), $\sigma(L^*) = \{d_1 < 0, , d_{N-1} < 0, d_N = 0\}$,
3. If $W^T L^* W = Diag(d_1, .., d_N)$, then $(w_r := \sum_s W_{rs} \dfrac{C_s}{||C_s||})_{r<N}$ orthonormal basis of $\mathbb{C}$, while $w_N \in \mathbb{K}$.

Remark : $\sigma(L^*[\mathcal{R}]) - (0) = \sigma(\mathcal{L}[\mathcal{R}]^{-1}_{|\mathbb{C}})$

$\Rightarrow$ Required properties on $\mathcal{L}[\mathcal{R}]$

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Setting the correct relaxation constraints

Alternative expressions for fluxes and $\mathcal{L}[\mathcal{R}]$:

$$\mathcal{L}[\mathcal{R}](g) = \sum_{j=1}^{N} \Phi_j \cdot \frac{\nabla p_j}{p_j} + kT A(V) : \sigma(u) + B'(v, I) \cdot \nabla(-\frac{1}{kT}) - \alpha(V, I) \nabla \cdot u,$$

with $A, B', \alpha \in \mathbb{C}^{\perp}$ and :

$$J_i = \sum_{j=1}^{N} k L_{ij}[\mathcal{R}] \frac{\nabla p_j}{p_j} + \theta_i[\mathcal{R}] T \nabla(-\frac{1}{kT}), \quad \theta_i T = \frac{1}{3} \left\langle \Phi_i, \mathcal{L}[\mathcal{R}]^{-1}(B') \right\rangle_{\mathcal{M}}.$$

Right constraints for the inverse problem:

$$\begin{cases} \langle \mathcal{R}(f), \phi_i \rangle = 0, 1 \leq i \leq N \\ \langle \mathcal{R}(f), w_r \rangle = -\lambda_r \langle f, w_r \rangle, \lambda_{r<N} = -d_{r<N}^{-1}, \\ \langle \mathcal{R}(f), \alpha \rangle = -\lambda \langle f, \alpha \rangle, \lambda = \dfrac{kT \|\alpha\|^2}{\eta_V^{exp}} \end{cases}$$

$\mathcal{L}[\mathcal{R}]^{-1}(B') \in \mathbb{C}^{\perp}$ $\Rightarrow$ right Fick coefficients.

$\lambda = \dfrac{kT \|\alpha\|^2}{\eta_V^{exp}}$ $\Rightarrow$ right second viscosity.

Construction of the relaxation operator

$$\mathcal{R}(f) = \nu(f)(G(f) - f)$$

Constraint set $K(f)$:

$$h \in \mathcal{K}(f) \Leftrightarrow \begin{cases} \langle h, \phi_i \rangle = \langle f, \phi_i \rangle, 1 \leq i \leq N \\ \langle h, w_r \rangle = -\lambda_r \langle f, w_r \rangle \\ \langle h, \alpha \rangle = -\lambda \langle f, \alpha \rangle \end{cases},$$

$$\mathcal{H}(f) = \langle f, \log f - 1 \rangle = \sum_i \iint f_i(\log f_i - 1) dv dI_i.$$

Extended phenomenological constraints set : $\tilde{\mathbb{C}} := \mathbb{C} \oplus \mathbb{R}\alpha$.
Entropy minimisation under constraints :
$\exists! G(f) = argmin_{g \in K(f)} \mathcal{H}(f)$ for $\nu \geq \max\{\lambda_r, r \leq N\} \cup \{\lambda\}$,

$$G_i(f) = n_i \left(\frac{m_i}{(2\pi k T^*_{tr})}\right)^{\frac{3}{2}} \left(\frac{1}{k T^*_{int}}\right)^{\frac{\delta_i}{2}} \Lambda_i^{-1} \exp\left(-\frac{m_i(v - u^*_i)^2}{2kT^*_{tr}} - \frac{I_i^{\frac{2}{\delta_i}}}{kT^*_{int}}\right)$$

Computations with the Fick relaxation operator

$$\boxed{\mathcal{L}[\mathcal{R}] = \nu(R \circ P_{\tilde{\mathbb{C}}} - P_{\mathbb{K}^\perp})}, \; R(w_r) = (1 - \frac{\lambda_r}{\nu})w_r, R(\alpha) = (1 - \frac{\lambda}{\nu})\alpha,$$

$$\boxed{\mathcal{L}^{-1}[\mathcal{R}] = \frac{1}{\nu}((R - Id)^{-1} \circ P_{\tilde{\mathbb{C}}} - P_{\tilde{\mathbb{C}}^\perp})}$$

- $\mathcal{R}$ is a well-defined operator,
- $L_{ij}[\mathcal{R}] = L_{ij}^{emp}$,
- $\eta = \frac{5nk^2T^2}{3\nu} = \eta^{emp}$, for $\nu := \frac{5nk^2T^2}{3\eta_{emp}}$,
- $\eta_V = \frac{2\delta nkT}{3\lambda(\delta+3)} = \eta_V^{emp}$.

$$\text{NSC} : \boxed{\eta^{emp} \leq \min\{\frac{5nk^2T^2}{3\max_r \lambda_r}, \frac{5}{6}(1 + \frac{3}{\delta})kT\eta_{emp}^V\}}.$$

Conclusions and perspectives

Conclusions :

- BGK model fulfilling **satisfying physics laws**, recovering **Fick law** and **both viscosities**,
- Possibility to adapt required quantities (from empirical values or any other operator's),
- Minimization obstacle while trying to recover extra coefficients,
- Generalization of monoatomic case.

Some perspectives :

- Include chemical reactions, conciliated with continuous model,
- Investigate possibility and modalities of containing mere monoatomic case (definition? $[\delta \to 0]$?),
- More realistic model, with $\delta = \delta(T)$.