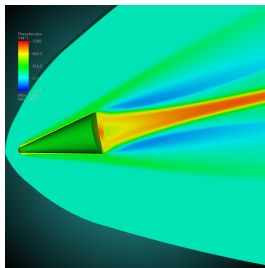


Moment models for rarefied gas dynamics at high temperatures

DE LA RECHERCHE À L'INDUSTRIE

cea



JULIEN MATHIAUD

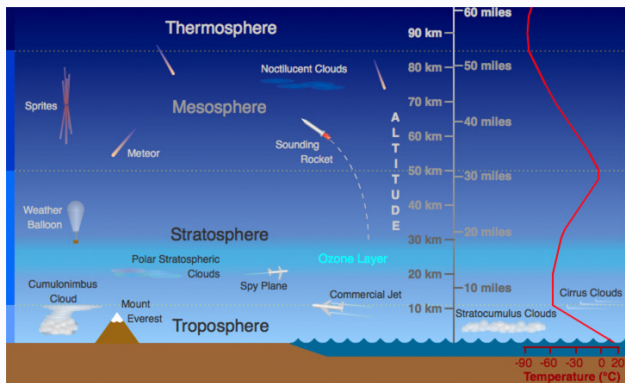
Joint work with L. Mieussens
CEA,CESTA / IMB / IPB (Bordeaux)

From rarefied flows to continuous flows

Rarefied Gas dynamics

Continuous laminar flows

Turbulent laminar flows

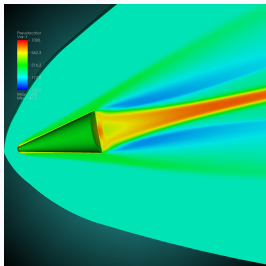


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- 2 New results for Fokker-Planck models
- 3 Models for vibrations
- 4 New results for BGK models and their extensions
- 5 Perspectives

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Steady flow

- Flow around spacecraft
- Hypersonic flows
- Sphere-cone configuration
- Quantities of interest: heat flux and aerodynamic coefficients

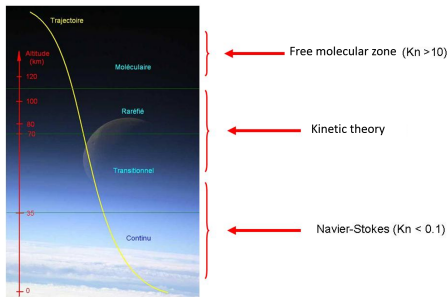


Looking for **steady state solution**: relaxation time scale \ll trajectory time scale

Knudsen number

Knudsen number:

$$Kn = \frac{\lambda}{L} \quad \left(\frac{\text{mean free path}}{\text{characteristic length}} \right)$$

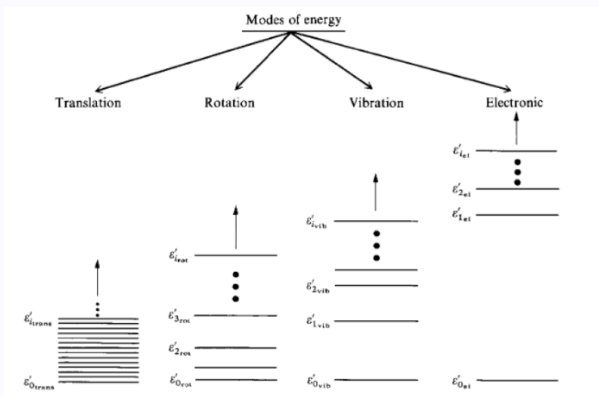


Prandtl number

The Prandtl number characterizes the ratio of the conductivity (λ) and the viscosity (μ) of a gas of specific heat C_p through: $Pr = \frac{\mu C_p}{\lambda}$.

In heat transfer problems, the Prandtl number controls the relative thickness of the momentum and thermal boundary layers. It is equal to $2/3$ for monoatomic perfect gases

Modes of energy in the air



	Translation	Rotation	Vibration	Electronic
Typical temperature of activation (K)	1	3	600	10000

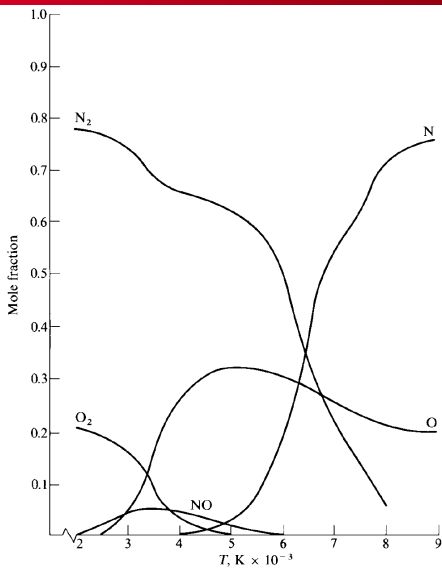


Fig. 11.12 Composition of equilibrium air vs temperature at 1 atm.

Boltzmann equation: $f(t, x, v)$

$$\partial_t f + v \cdot \nabla_x f = Q(f, f),$$

$$Q(f, f)(v) = \iint_{v_* \in \mathbb{R}^3, \sigma \in \mathbb{S}^2} \left(f(v'_*) f(v') - f(v_*) f(v) \right) r^2 |v - v_*| d\sigma dv_*,$$

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma \quad , \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma.$$

Advantages and drawbacks

- + Capture the correct physics: in the Chapman expansion one recovers the Prandtl number of Navier-Stokes equation which is equal to $\frac{2}{3}$ for a monoatomic gas
- High numerical cost in transitional area between 100km and 60km (6D non linear problem).

BGK equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau} (M(f) - f),$$

$M(f) = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{|v-u|^2}{2RT}\right)$ is the Maxwellian of equilibrium satisfying:

$$\langle f \rangle = \int f dv = \rho, \langle fv \rangle = \int f v dv = \rho u, \langle f \frac{1}{2}(v-u)^2 \rangle = \int f \frac{1}{2}(v-u)^2 dv = \frac{3}{2} \rho T$$

τ : characteristic time of collisions.

Fokker Planck equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau} \nabla_v \cdot ((v-u)f + T \nabla_v f),$$

Advantages and drawbacks

- Physics only approximated: thermal flux underestimated. The Prandtl number is equal to 1 for BGK model and $\frac{3}{2}$ for *FP* model.
- + Numerical cost less important in transitional area between 100km and 60km.

How to recover the correct Prandtl number?

For BGK models it has been done using the ESBGK model:

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau} (G(f) - f),$$

with $G(f)$ anisotropic Gaussian defined as:

$$G(f) = \frac{\rho}{\sqrt{\det(2\pi\Pi)}} \exp\left(-\frac{(v-u)\Pi^{-1}(v-u)}{2}\right).$$

Π being a tensor linked to the different temperatures of thermal agitation.

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Equations

We consider a gas described by the particle mass density $f(t, x, v, I)$ that at time t have the position x , the velocity v and an internal energy parameter I (of internal energy $I^{2/\delta}$):

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau} \underbrace{\left(\nabla_v \cdot ((v - u)f + \Pi \nabla_v f) + \partial_I (\delta f I + \frac{\delta^2}{2} RT_{rel} I^{2-\frac{2}{\delta}} \partial_I f) \right)}_{D(f)},$$

with:

$$\Theta := \frac{1}{\rho} \langle (v - u) \otimes (v - u) f \rangle,$$

$$E_{tr} = \frac{3}{2} \rho RT_{tr} = \langle \frac{1}{2} |v - u|^2 f \rangle, \quad E_{int} = \frac{\delta}{2} \rho RT_{int} = \langle \varepsilon(I) f \rangle,$$

$$T = \frac{3}{3 + \delta} T_{tr} + \frac{\delta}{3 + \delta} T_{int},$$

$$\Pi = (1 - \theta) ((1 - \nu) RT_{tr} Id + \nu \Theta) + \theta RT Id,$$

$$T_{rel} = (1 - \theta) T_{int} + \theta T.$$

where the coefficients ν and θ are some free parameters to be fitted.

Proposition

We assume ν satisfies a positiveness condition for Π and that $\nu < 1$. The collision operator D conserves mass, momentum, and energy:

$$\left\langle (1, \nu, \frac{1}{2}|v|^2 + I^{2/\delta}) D(f) \right\rangle = 0,$$

It satisfies the dissipation of the entropy:

$$\langle D(f) \log f \rangle \leq 0,$$

and the equilibrium property:

$$D(f) = 0 \Leftrightarrow f = G_p(f) \Leftrightarrow f = M_p(f).$$

with:
$$M_p(f) = \frac{\rho \Lambda_\delta}{(2\pi)^{3/2} (RT)^{(3+\delta)/2}} \exp\left(-\frac{|v-u|^2}{2RT} - \frac{I^{2/\delta}}{RT}\right),$$

$$G_p(f) = \frac{\rho \Lambda_\delta}{\sqrt{\det(2\pi\Pi)} (RT_{rel})^{\delta/2}} \exp\left(-\frac{1}{2} \begin{pmatrix} v-u \\ \delta I \end{pmatrix}^T \begin{pmatrix} \Pi & 0 \\ 0 & \frac{\delta^2}{2} RT_{rel} I^{2-\frac{2}{\delta}} \end{pmatrix}^{-1} \begin{pmatrix} v-u \\ \delta I \end{pmatrix}\right).$$

Navier-Stokes limit through Chapman-Enskog expansion

The moments of f satisfy, up to $O(Kn^2)$, the Navier-Stokes equations:

$$\partial_t \rho + \nabla \cdot \rho u = 0,$$

$$\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p = -\nabla \cdot \sigma,$$

$$\partial_t E + \nabla \cdot (E + p)u = -\nabla \cdot q - \nabla \cdot (\sigma u),$$

where the shear stress tensor and the heat flux are given by

$$\sigma = -\mu(\nabla u + (\nabla u)^T - \alpha \nabla \cdot u), \quad \text{and} \quad q = -\kappa \nabla \cdot T,$$

with the following values of the viscosity and heat transfer coefficients (in dimensional variables).

$$\mu = \frac{\tau p}{2(1 - (1 - \theta)\nu)}, \quad \alpha = (\gamma - 1) - \frac{(1 - \nu)(1 - \theta)}{\theta} \left(\frac{5}{3} - \gamma \right) \quad \text{and} \quad \kappa = \frac{5 + \delta}{6} \tau p R,$$

and $\gamma = \frac{\delta + 5}{\delta + 3}$. Moreover, the corresponding Prandtl number is

$$\text{Pr} = 3 / (2(1 - (1 - \theta)\nu)).$$

Ornstein-Uhlenbeck process

The Ornstein-Uhlenbeck process reads:

$$dV_i(t) = -\frac{dt}{\tau} (V_i(t) - u) + A_v dB_v(t),$$

$$d\varepsilon_i(t) = -\frac{2dt}{\tau} \left(\varepsilon_i(t) - \frac{\delta}{2} RT_{rel} \right) + 2\sqrt{RT_{rel}\varepsilon_i(t)} dB_\varepsilon(t),$$

$$V_i^{n+1} = \left(1 - \frac{\Delta t}{\tau} \right) (V_i^n - u) + \sqrt{\frac{2\Delta t}{\tau}} A \begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix}$$

$$\varepsilon_i^{n+1} = \left(\left(\sqrt{\varepsilon_i^n} + \sqrt{\frac{dt}{\tau} RT_{rel} B_\varepsilon} \right)^2 + (\delta - 1) RT_{rel} \frac{dt}{\tau} \right) / \left(1 + \frac{2dt}{\tau} \right),$$

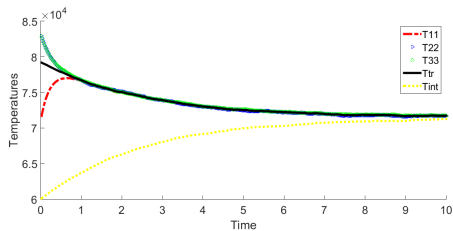


Figure: Convergence of the directional translational temperatures and the internal temperature to their equilibrium value.

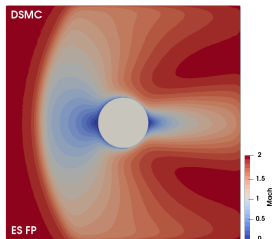


Figure: Comparison at Mach 2, $Kn=0.05$ between DSMC and FP in collaboration with H. Gorji (RWTH Aachen, Germany)

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Definition

Let $f(t, x, v, \varepsilon, i)$ be the mass density distribution of particles with position x , velocity v , internal energy ε , and in the i -th vibrational energy level, such that its vibrational energy is iRT_0 (T_0 : characteristic vibrational temperature of the molecule). The corresponding local equilibrium distribution is defined by:

$$M_{vib}[f](v, \varepsilon, i) = \frac{\rho}{\sqrt{2\pi RT}^3} \frac{1 - e^{-T_0/T}}{RT} \exp\left(-\frac{\frac{1}{2}|u - v|^2 + \varepsilon + iRT_0}{RT}\right)$$

$$\rho = \langle f \rangle_{v,\varepsilon,i}, \quad \rho u = \langle vf \rangle_{v,\varepsilon,i}, \quad \rho e = \left\langle \left(\frac{1}{2}|v - u|^2 + \varepsilon + iRT_0 \right) f \right\rangle_{v,\varepsilon,i},$$

where we use the notation $\langle \phi \rangle_{v,\varepsilon,i} = \sum_{i=0}^{\infty} \iint \phi(t, x, v, \varepsilon, i) dv d\varepsilon$ for any function ϕ .

The temperature T can be recovered by inverting the relation $e = \left(\frac{5}{2} + \frac{T_0/T}{e^{T_0/T} - 1} \right) RT$ so that there exists T^{-1} such that $T = T^{-1}(e)$.

The entropy $H(f)$ of f is naturally defined through $H(f) = \langle f \log f \rangle_{v,\varepsilon,i}$.

Properties of the equilibrium

$$\langle M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho, \quad \langle vM_{vib}[f] \rangle_{v,\varepsilon,i} = \rho u, \quad \left\langle \left(\frac{1}{2}(v-u)^2 + \varepsilon + iRT_0 \right) M_{vib}[f] \right\rangle_{v,\varepsilon,i} = \rho e.$$

Energies at equilibrium

At equilibrium, we define the following energies of translation, rotation, and vibration:

$$e_{tr}(T) = \left\langle \left(\frac{1}{2}(v-u)^2 \right) M_{vib}[f] \right\rangle_{v,\varepsilon,i} = \frac{3}{2} \rho RT, \quad (1)$$

$$e_{rot}(T) = \langle \varepsilon M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho RT, \quad (2)$$

$$e_{vib}(T) = \langle (iRT_0) M_{vib}[f] \rangle_{v,\varepsilon,i} = \rho \frac{RT_0}{e^{T_0/T} - 1} = \rho \frac{\delta(T)}{2} RT, \quad (3)$$

with $\delta(T) = 2 \frac{T_0/T}{e^{T_0/T} - 1}$.

Reduced distributions

For computational efficiency, it is interesting to define marginal, or reduced, distributions F and G by :

$$F(t, x, v, \varepsilon) = \sum_i f(t, x, v, \varepsilon, i),$$

$$G(t, x, v, \varepsilon) = \sum_i iRT_0 f(t, x, v, \varepsilon, i).$$

The macroscopic variables defined by f can be obtained through F and G only

$$\rho = \langle F \rangle_{v,\varepsilon}, \quad \rho u = \langle vF \rangle_{v,\varepsilon}, \quad \rho e = \left\langle \left(\frac{1}{2}(v-u)^2 + \varepsilon \right) F \right\rangle_{v,\varepsilon} + \langle G \rangle_{v,\varepsilon}.$$

where we use the notation $\langle \psi \rangle_{v,\varepsilon} = \iint \psi(t, x, v, \varepsilon) dv d\varepsilon$ for any function ψ .

Entropy

The reduced entropy $\mathcal{H}(F, G)$ of the system is:

$$\mathcal{H}(F, G) = \left\langle F \log(F) + F \log \left(\frac{RT_0 F}{RT_0 F + G} \right) + \frac{G}{RT_0} \log \left(\frac{G}{RT_0 F + G} \right) \right\rangle_{v, \varepsilon}.$$

Proof (1)

The set $\{f > 0 \text{ such that } \sum_i f_i = F, \sum_i iRT_0 f_i = G\}$ is clearly convex, so that we can use a Lagrangian multiplier approach by finding a saddle point of the function \mathcal{I} defined through :

$$\mathcal{I}(f, \alpha, \beta) = \sum_i f_i \log f_i - \alpha \left(\sum_i f_i - F \right) - \beta \left(\sum_i iRT_0 f_i - G \right),$$

where α and β are real numbers.

Proof (2)

The saddle point satisfies $\frac{\partial \mathcal{I}}{\partial f} = 0$, and one deduces that f can be written $f_i(\nu, \varepsilon) = A(\nu, \varepsilon) \exp(-iB(\nu, \varepsilon)T_0)$. The linear constraints give:

$$F = \sum_i f_i = \frac{A}{1 - \exp(-BT_0)} \quad , \quad G = \sum_i f_i iRT_0 = \frac{ART_0 \exp(-BT_0)}{(1 - \exp(-BT_0))^2}.$$

Solving this linear system gives:

$$H(F, G) = F \log(F) + F \log\left(\frac{RT_0 F}{RT_0 F + G}\right) + \frac{G}{RT_0} \log\left(\frac{G}{RT_0 F + G}\right),$$

using that $G/F = e_{vib}(1/B)$.

A final integration with respect to ν and ε gives the final result:

$$\mathcal{H}(F, G) = \langle H(F, G) \rangle_{\nu, \varepsilon}$$

Proposition

We have the following properties

- the function $(F, G) \mapsto H(F, G)$ is convex.
- the minimum of $\mathcal{H}(F_1, G_1)$ on \mathcal{S} is obtained on $(M_{vib}(F, G), N_{vib}(F, G))$ with:

$$M_{vib}(F, G) = \frac{\rho}{\sqrt{2\pi RT^3}} \exp\left(-\frac{\rho|u-v|^2}{2RT}\right) \frac{1}{RT} \exp\left(-\frac{\varepsilon}{RT}\right),$$

$$N_{vib}(F, G) = e_{vib}(T)M_{vib}(F, G),$$

where $e_{vib}(T)$ is the equilibrium vibrational energy.

Properties

- We note $\mathbb{H}(F, G)$ be the positive-definite Hessian matrix of H .

$$\mathbb{H}(F, G) = \begin{pmatrix} \frac{2}{F} - \frac{RT_0}{RT_0 F + G} & -\frac{1}{RT_0 F + G} \\ -\frac{1}{RT_0 F + G} & \frac{F}{G(RT_0 F + G)} \end{pmatrix} \quad (4)$$

It satisfies: $1 = FH_{11}(F, G) + GH_{21}(F, G)$, $0 = FH_{12}(F, G) + GH_{22}(F, G)$.

- Using $D_1(H)(F, G) = 1 + \log\left(\frac{RT_0 F^2}{RT_0 F + G}\right)$, $D_2(H)(F, G) = \frac{1}{RT_0} \log\left(\frac{G}{RT_0 F + G}\right)$, we have:

$$\begin{aligned} & \mathcal{H}(M_{vib}(F, G), N_{vib}(F, G)) - \mathcal{H}(F, G) \\ & \geq D_1(H)(F, G)(M_{vib}(F, G) - F) + D_2(H)(F, G)(N_{vib}(F, G) - G) \end{aligned} \quad (5)$$

Consequences

Equations (4) and (5) respectively give the second principle for the Fokker-Planck model and the BGK model we are going to construct.

Model

$$\begin{aligned}\partial_t F + v \cdot \nabla_x F &= \frac{1}{\tau} (M_{vib}[F, G] - F), \\ \partial_t G + v \cdot \nabla_x G &= \frac{1}{\tau} (N_{vib}[F, G] - G).\end{aligned}$$

with:

$$\begin{aligned}F &= \sum_i f(t, x, v, \varepsilon, i), \quad G = \sum_i iRT_0 f(t, x, v, \varepsilon, i), \\ M_{vib}[F, G] &= \frac{\rho}{\sqrt{2\pi RT}^3} \exp\left(-\frac{\rho|u-v|^2}{2\rho}\right) \frac{1}{RT} \exp\left(-\frac{\varepsilon}{RT}\right), \\ \rho &= \langle F \rangle_{v,\varepsilon}, \quad \rho u = \langle Fv \rangle_{v,\varepsilon}, \quad \rho e = \left\langle F \left(\frac{1}{2}(v-u)^2 + \varepsilon \right) \right\rangle_{v,\varepsilon} + \langle G \rangle_{v,\varepsilon}, \\ T &= T^{-1}(e).\end{aligned}$$

Hydrodynamic limit

Let (F, G) be solutions of BGK equations up to $O(\text{Kn}^2)$. Then the moments of (F, G) satisfy the following Navier-Stokes equations up to $O(\text{Kn}^2)$:

$$\begin{cases} \partial_t \rho + \text{div}_{\mathbf{x}}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \text{div}_{\mathbf{x}}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} p = -\text{div}_{\mathbf{x}}(\sigma) + O(\text{Kn}^2) \\ \partial_t E + \text{div}_{\mathbf{x}}((E + p)\mathbf{u}) = -\text{div}_{\mathbf{x}}(\mathbf{q}) - \text{div}_{\mathbf{x}}(\sigma \mathbf{u}) + O(\text{Kn}^2), \end{cases}$$

with:
$$E = \left\langle \left(\frac{1}{2} |v|^2 + \varepsilon \right) F + G \right\rangle_{v, \varepsilon} = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2,$$

$$\sigma = -\mu \left(\nabla_{\mathbf{x}} \mathbf{u} + \nabla_{\mathbf{x}} \mathbf{u}^T - \mathcal{C} \text{div}_{\mathbf{x}}(\mathbf{u}) \text{Id} \right),$$

$$\mathbf{q} = -\mu \nabla_{\mathbf{x}} h,$$

where $h = e + RT$, $\mathcal{C} = \partial_e(RT) = \frac{R}{C_v(T)}$, $C_v(T) = \frac{5}{2}R + \frac{(T_0/T)^2 e^{T_0/T}}{(e^{T_0/T} - 1)^2} R$.

By defining $C_p = C_v + R$ the specific heat at constant pressure, one gets:

$$\mathbf{q} = -\mu C_p \nabla_{\mathbf{x}} T,$$

so that as usual only a gas with a Prandtl number of one is obtained.

Model

$$\partial_t F + v \cdot \nabla_x F = D_F(F, G),$$

$$\partial_t G + v \cdot \nabla_x G = D_G(F, G).$$

with:

$$F = \sum_i f(t, x, v, \varepsilon, i), \quad G = \sum_i iRT_0 f(t, x, v, \varepsilon, i),$$

$$D_F(F, G) = \frac{1}{\tau} (\nabla_v \cdot ((v - u)F + T\nabla_v F) + 2\nabla_\varepsilon (F\varepsilon + RT\varepsilon\nabla_\varepsilon F)),$$

$$D_G(F, G) = \frac{1}{\tau} (\nabla_v \cdot ((v - u)G + T\nabla_v G) + 2\nabla_\varepsilon (G\varepsilon + RT\varepsilon\nabla_\varepsilon G))$$

$$+ \frac{2}{\tau} (e_{vib}(T)F - G),$$

$$\rho = \langle F \rangle_{v,\varepsilon}, \quad \rho u = \langle Fv \rangle_{v,\varepsilon}, \quad \rho e = \left\langle F \left(\frac{1}{2}(v - u)^2 + \varepsilon \right) \right\rangle_{v,\varepsilon} + \langle G \rangle_{v,\varepsilon},$$

$$T = T^{-1}(e).$$

Hydrodynamic limit

Let (F, G) be solutions of BGK equations up to $O(\text{Kn}^2)$. Then the moments of (F, G) satisfy the following Navier-Stokes equations up to $O(\text{Kn}^2)$:

$$\begin{cases} \partial_t \rho + \text{div}_{\mathbf{x}}(\rho u) = 0 \\ \partial_t(\rho u) + \text{div}_{\mathbf{x}}(\rho u \otimes u) + \nabla_x p = -\text{div}_{\mathbf{x}}(\sigma) + O(\text{Kn}^2) \\ \partial_t E + \text{div}_{\mathbf{x}}((E + p)u) = -\text{div}_{\mathbf{x}}(q) - \text{div}_{\mathbf{x}}(\sigma u) + O(\text{Kn}^2), \end{cases}$$

with:

$$E = \left\langle \left(\frac{1}{2} |v|^2 + \varepsilon \right) F + G \right\rangle_{v, \varepsilon} = \rho e + \frac{1}{2} \rho |u|^2,$$

$$\sigma = -\mu \left(\nabla_x u + \nabla_x u^T - \mathcal{C} \text{div}_{\mathbf{x}}(u) \text{Id} \right), \quad q = -\frac{2}{3} \mu \nabla_x h,$$

where $h = e + RT$, $\mathcal{C} = \partial_e(RT) = \frac{R}{C_v(T)}$, $C_v(T) = \frac{5}{2}R + \frac{(T_0/T)^2 e^{T_0/T}}{(e^{T_0/T} - 1)^2} R$.

By defining $C_p = C_v + R$ the specific heat at constant pressure, one gets:

$$q = -\frac{2}{3} \mu C_p \nabla_x T,$$

so that as usual only a gas with a Prandtl number of $3/2$ is obtained.

Recovering Prandtl number: the easy part

As usual there is a need for a Gaussian equilibrium to correct the characteristics times of relaxation . So we will need to go to an ESGK or an ESFP model...

Recovering Prandtl number: the tricky part

Since relaxation times for rotation and vibration are not of the same order there is a need for a model with more equations (3 probably) to capture correctly the relaxation phenomena: the Prandtl number cannot be the only criterion to correct the model.

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Equations

$$\partial_t f + v \cdot \nabla f = \frac{M[f] - f}{\tau}, \quad (6)$$

where the Maxwellian equilibrium is $M[f] = M[\rho, u, e]$ defined by

$$M[f](v, \varepsilon) = \frac{\rho}{\sqrt{2\pi} \frac{\rho}{\rho}}^3 \exp\left(-\frac{\rho|u-v|^2}{2\rho}\right) \Lambda(\delta) \left(\frac{\rho\varepsilon}{\rho}\right)^{\frac{\delta}{2}-1} \frac{\rho}{\rho} \exp\left(-\frac{\rho\varepsilon}{\rho(\rho, e)}\right).$$

The macroscopic quantities are given by

$$\begin{aligned} \rho &= \langle\langle f \rangle\rangle, \\ u &= \frac{1}{\rho} \langle\langle fv \rangle\rangle, \\ e &= \frac{1}{\rho} \langle\langle \left(\frac{|v-u|^2}{2} + \varepsilon \right) f \rangle\rangle, \end{aligned}$$

with $\langle\langle \cdot \rangle\rangle = \iint_{\mathbb{R}^3 \times \mathbb{R}^+} \cdot \, dv d\varepsilon$, and the closure relation on the pressure $p = p(\rho, e)$.

Prandtl and Schmidt numbers

Let f be the solution of BGK equation up to $O(\text{Kn}^2)$. Its moments satisfy the following Navier-Stokes equations up to $O(\text{Kn}^2)$:

$$\begin{cases} \partial_t \rho + \text{div}_{\mathbf{x}}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \text{div}_{\mathbf{x}}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla_x \mathbf{p} = -\text{div}_{\mathbf{x}}(\boldsymbol{\sigma}) + O(\text{Kn}^2) \\ \partial_t \mathbf{E} + \text{div}_{\mathbf{x}}((\mathbf{E} + \mathbf{p}) \mathbf{u}) = -\text{div}_{\mathbf{x}}(\mathbf{q}) - \text{div}_{\mathbf{x}}(\boldsymbol{\sigma} \mathbf{u}) + O(\text{Kn}^2), \end{cases}$$

with: $\mathbf{E} = \rho \mathbf{e} + \frac{1}{2} \rho |\mathbf{u}|^2$, $\boldsymbol{\sigma} = -\mu \left(\nabla_x \mathbf{u} + \nabla_x \mathbf{u}^T - \mathcal{C} \text{div}_{\mathbf{x}}(\mathbf{u}) \text{Id} \right)$, $\mathbf{q} = -\mu \nabla_x h$.

$$h = \mathbf{e} + \mathbf{p} / \rho \quad , \quad \mathcal{C} = \frac{\rho}{\rho} \left(\partial_1 \mathbf{p} + \frac{\rho}{\rho^2} \partial_2 \mathbf{p} - \frac{\rho}{\rho} \right).$$

For reacting perfect gases at equilibrium $h(\rho, T) = \sum_i c_i(\rho, T) h_i(T)$ with c_i mass concentration of the i -th gas and h_i its enthalpy. We get that:

$$\mu \nabla h = \mu \left(\left(\sum_i c_i c_{\rho_i} \right) \nabla T + \sum_i h_i(T) \nabla c_i \right).$$

The Prandtl number is equal to **one**. We also note that D_i the multicomponent diffusion coefficient of the i th component is $\frac{\mu}{\rho}$ so that the Schmidt number $\frac{\mu}{\rho D_i}$ is equal to **one**.

Mach 10, Knudsen 0.1

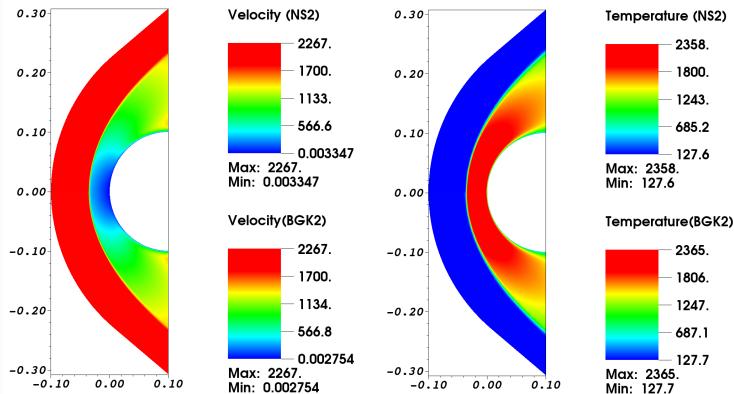


Figure: Velocity field and Temperature field (Top:Navier-Stokes solver NS2, bottom: new model BGK2)

Mach 10, Knudsen 0.1

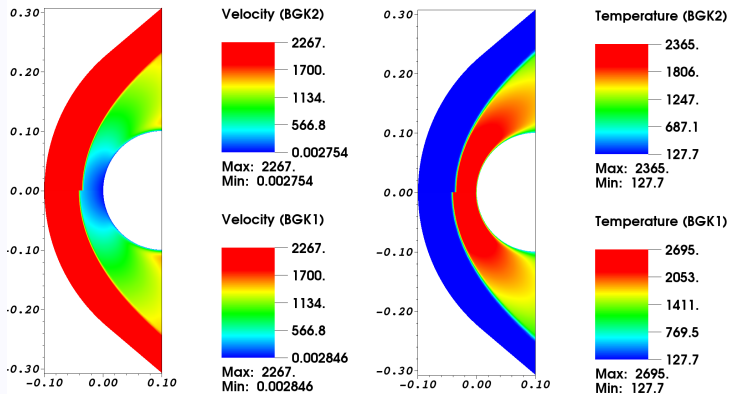


Figure: Velocity field and Temperature field (Top: new model BGK2, bottom: old model BGK1)

Mach 10, Knudsen 0.1

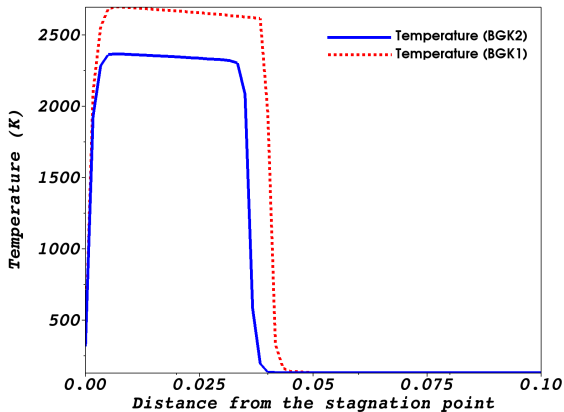


Figure: Temperature along the axis

Notations

For every species of the mixture, numbered with index i :

- its concentration c_i depends on ρ and e only: $c_i = c_i(\rho, e)$;
- its pressure p_i satisfies the usual perfect gas law: $p_i = \rho_i R_i T$, where R_i is the gas constant of the species and $\rho_i = c_i(\rho, e)\rho$, so that $p_i = p_i(\rho, e)$;
- its specific energy e_i and enthalpy h_i depend on T only: $e_i = e_i(T)$ and $h_i = h_i(T)$, where $e_i(T) = \frac{3+\delta_i(T)}{2} R_i T + e_i^{f,0}$, with $e_i^{f,0}$ is the energy of formation of the i th molecule and $\delta_i(T)$ is the number of activated internal degrees of freedom of the molecule that might depend on the temperature, see the previous sections.

For compressible Navier-Stokes equations for an equilibrium chemically reacting mixture, these quantities are not necessary. Instead, it is sufficient to define (with analytic formulas or tables):

- the total pressure $p = \sum_i p_i(\rho, e)$ so that $p = p(\rho, e) = \rho R(\rho, e) T$, with $R(\rho, e) = \sum_i c_i(\rho, e) R_i$;
- the temperature T , though the relation $e = \sum_i c_i(\rho, e) e_i(T)$, so that $T = T(\rho, e)$;
- the total specific enthalpy $h = \sum_i c_i h_i$, so that $h = h(\rho, e) = e + \frac{p(\rho, e)}{\rho}$.

Equations

$$\begin{aligned} \partial_t f + v \cdot \nabla_x f &= \frac{1}{\tau} (MGE[f, g] - f), \text{ with: } MGE[f, g] = \sum_{1 \leq i \leq N} M_i[f, g] \\ \partial_t g + v \cdot \nabla_x g &= \frac{1}{\tau} (NMGE[f, g] - g), \text{ with: } NMGE[f, g] = \sum_{N_m+1 \leq i \leq N} N_i[f, g] \end{aligned} \quad (7)$$

with the following definitions for reduced Maxwellians:

$$\text{for } 1 \leq i \leq N, M_i[f, g] = \frac{\rho c_i}{(2\pi R_i T)^{\frac{3}{2}}} \exp\left(-\frac{|v-u|^2}{2R_i T}\right),$$

$$\text{for } N_m + 1 \leq i \leq N, N_i[f, g] = \left(\frac{\delta_i(T)}{2} R_i T + e_i^{f,0}\right) \frac{\rho c_i}{(2\pi R_i T)^{\frac{3}{2}}} \exp\left(-\frac{|v-u|^2}{2R_i T}\right),$$

Closure

We define $c_i(\rho, e)$ as the mass concentration of i -th molecule, $T := T(\rho, e)$ as the mean temperature depending on internal energy and density which are defined through the following relations:

$$\begin{aligned}\rho(t, x) &= \int_{\mathbb{R}^3} f \, dv = \int_{\mathbb{R}^3} MGE[f, g] \, dv \\ \rho u(t, x) &= \int_{\mathbb{R}^3} v f \, dv = \int_{\mathbb{R}^3} v MGE[f, g] \, dv, \\ \rho e(t, x) &= \int_{\mathbb{R}^3} \left(\frac{1}{2} |v - u|^2 f + g \right) dv, \\ &= \int_{\mathbb{R}^3} \left(\frac{1}{2} |v - u|^2 MGE[f, g] + NMGE[f, g] \right) dv\end{aligned}$$

Through the "real gas closure" we have:

$e = \sum_{1 \leq i \leq N_m + N_d} c_i(\rho, e) \left(\frac{3 + \delta_i(T(\rho, e))}{2} R_i T(\rho, e) + e_i^{f,0} \right)$, where $e_i^{f,0}$ is the energy of formation of the i -th molecule and δ_i the number of activated degrees of freedom of this molecule ($\delta_i = 0$ for $i \leq N_m$).

NS equations

The moments of f, g , solution of the MGE model (7), satisfy the following Navier-Stokes equations, up to $O(\text{Kn}^2)$:

$$\begin{aligned}
 \partial_t \rho + \nabla \cdot \rho \mathbf{u} &= 0, \\
 \partial_t \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p &= -\nabla \cdot \boldsymbol{\sigma}, \\
 \partial_t E + \nabla \cdot (E + p)\mathbf{u} &= -\nabla \cdot \mathbf{q} - \nabla \cdot (\boldsymbol{\sigma} \mathbf{u}),
 \end{aligned} \tag{8}$$

where Kn is the Knudsen number (defined below), E is the total energy density defined by $E = \left\langle \left\langle \left(\frac{1}{2} |v|^2 + \varepsilon \right) F \right\rangle \right\rangle = \frac{1}{2} \rho |u|^2 + \rho e$.

NS equations

σ and q are the shear stress tensor and heat flux vector defined by

$$\sigma = -\mu \left(\nabla u + (\nabla u)^T + (1 - C_p) \nabla \cdot u \text{Id} \right),$$

$$q = -\mu \left(\frac{\sum_i c_i R_i c_p^i + \sum_{i < j} c_i c_j \frac{(h_i - h_j)^2}{T^2}}{\sum_i c_i R_i} \right) \nabla T - \mu \sum_{i < j} \frac{c_i c_j}{\sum_i c_i R_i} (h_i - h_j) \nabla \left(\frac{\mu_i - \mu_j}{T} \right).$$

with $h_i = e_i + R_i T(\rho, e)$ is the enthalpy, $\mu_i := \mu_i(\rho, e)$ is the mass chemical potential of the i -th specie depending on ρ and e (we recall that μ defines the viscosity and not a chemical potential), and $C_p = \frac{\rho}{\rho} \partial_\rho \rho + \frac{\rho}{\rho} \frac{\partial e \rho}{\rho}$

Some remarks

- if $N_m + N_d = 1$, we recover the classical BGK model for monoatomic or polyatomic model with two distributions so that we capture the correct hydrodynamic limit with a Prandtl number of one.
- We are still unable to prove something close to a second principle for such a model even if it can capture more physics like equilibrium of two inert gases.
- The role of chemical potential in the formula is still under investigation: this term does not appear for classical Navier-Stokes equations for Atmospheric reentry with a "real gas" closure but it appears under various forms in papers for kinetic mixtures models and is linked to Onsager's relations ($\frac{1}{T}$ and $-\frac{u_j}{T}$ are conjugate variables for u and ρ).

- 1 Context
- 2 New results for Fokker-Planck models
- 3 Models for vibrations
- 4 New results for BGK models and their extensions
- 5 Perspectives**

Numeric

- Testing the BGK model with a law of real gas
- Pursuing tests on Fokker-Planck Models

Models

- Capturing the different relaxation times for energies,
- Going to non equilibrium chemistry with a "simple model"

- [[Bar + 18](#)] Baranger,C., Marois,G., Mathé,J., Mathiaud, J. and Mieussens,L. “A BGK model for high temperature rarefied gas flows”. In: Work in progress (2018).
- [[MM16](#)] J. Mathiaud and L. Mieussens. “A Fokker–Planck Model of the Boltzmann Equation with Correct Prandtl Number”. In: Journal of Statistical Physics 162.2 (Jan. 2016), pp. 397–414.
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- [[MM18](#)] J. Mathiaud and L. Mieussens. “Vibrational models of Boltzmann equation with correct second principle: BGK and Fokker-Planck”. In: Work in progress (2018).