DE LA RECHERCHE À L'INDUSTRIE

A new diffusive model for rarefied gas dynamics

Julien Mathiaud (CEA/CESTA),
Luc Mieussens (IMB)

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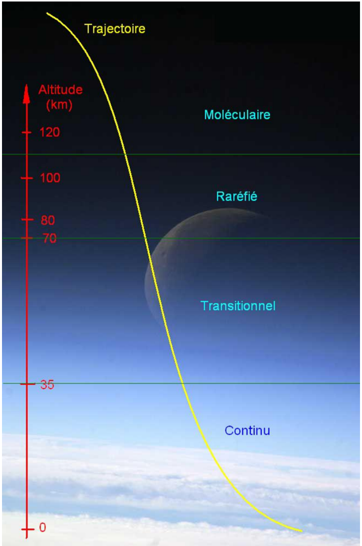
Plan

Context and objectives



Objectives

- Capture the correct thermal fluxes in order to design re-entry vehicles,
- Use a kinetic model able to recover Navier-Stokes equations in its hydrodynamic limit to ensure a continuity in models.
- One key point is to recover the correct Prandtl number:

$$\mathrm{Pr} = \frac{\gamma R}{\gamma - 1} \frac{\mu}{\kappa}$$

(equal to $\frac{2}{3}$ for monoatomic gases) .

Zoology of models (1): Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = Q(f, f), \tag{1}$$

with

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

and

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

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

Advantages and drawbacks

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

Zoology of models (2): BGK equation and Fokker Planck equation

BGK equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau}\left(M(f) - f\right), \tag{2}$$

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

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

τ: characteristic time of collisions.

Fokker Planck equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau}\nabla_v \cdot \left((v-u)f + T\nabla_v f\right), \tag{3}$$

Zoology of models (2): BGK equation and Fokker Planck equation

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:

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau}\left(G(f) - f\right), \tag{4}$$

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.

Equation of the ESFP model (1)

The model is the following:

$$\partial_t f + v \cdot \nabla_x f = D(f), \tag{5}$$

where the collision operator is defined by

$$D(f) = \frac{1}{\tau} \nabla_v \cdot \left((v-u) f + \Pi \nabla_v f \right), \tag{6}$$

where τ is a relaxation time, and Π is a convex combination between the temperature tensor Θ and its equilibrium value RTI, that is to say:

$$\Pi = (1-\nu) RTI + \nu \Theta, \tag{7}$$

with ν parameter to be set and

$$\Theta := \frac{1}{\rho} \left\langle (v-u) \otimes (v-u) f \right\rangle. \tag{8}$$

Other formulations for ESFP

The operator D has two other equivalent formulations:

$$D(f) = \frac{1}{\tau}\nabla_v \cdot \left(\Pi G(f) \nabla_v \frac{f}{G(f)}\right), \tag{9}$$

and

$$D(f) = \frac{1}{\tau}\nabla_v \cdot \left(\Pi f \nabla_v \log\left(\frac{f}{G(f)}\right)\right), \tag{10}$$

where $G(f)$ is the anisotropic Gaussian defined by

$$G(f) = \frac{\rho}{\sqrt{\det(2\pi\Pi)}} \exp\left(-\frac{(v-u)\Pi^{-1}(v-u)}{2}\right), \tag{11}$$

which has the same 5 first moments as f

$$\left\langle (1, v, \tfrac{1}{2}|v|^2) G(f) \right\rangle = (\rho, \rho u, E),$$

and has the temperature tensor $\langle (v-u) \otimes (v-u) G(f) \rangle = \Pi$.

Validity of the model according to the ν parameter

Condition of strict positiveness of Π

The tensor Π is symmetric positive definite for every tensor Θ if, and only if,

$$-\frac{RT}{\lambda_{max} - RT} < \nu < \frac{RT}{RT - \lambda_{min}}, \tag{12}$$

where λ_{max} and λ_{min} are the (positive) maximum and minimum eigenvalues of Θ.

Moreover Π is unconditionally definite positive with respect to the eigenvalues of Θ as long as :

$$-\frac{1}{2} < \nu < 1. \tag{13}$$

Kinetic properties of the model:

Conservation

We suppose that the condition of strict positiveness (equations 12) is fulfilled by ν. The operator D conserves the mass, momentum, and energy:

$$\left\langle (1, v, \tfrac{1}{2}|v|^2) D(f) \right\rangle = 0.$$

Entropy decay

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

Equilibrium

$$D(f) = 0 \Leftrightarrow f = G(f) \Leftrightarrow f = M(f).$$

Chapman Enskog expansion

Non dimensional ESFP equation

Assume we have some reference values of length x, pressure p, and temperature T.
We can derive reference values for all the other quantities: mass density $\rho = p/RT$, velocity $v = \sqrt{RT}$, time $t_* = x/v$, distribution function $f = \rho/(RT)^{3/2}$. We also assume we have a reference value for the relaxation time τ.

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} D(f), \tag{14}$$

where $\varepsilon = \frac{v\tau}{x}$ is the Knudsen number.

Main result of the Chapman-Enskog analysis (1)

The solution of the ESFP model satisfies, up to $O(\varepsilon^2)$ the Navier-Stokes equations (ε being the Knudsen number defined below):

$$\begin{aligned} &\partial_t \rho + \nabla \cdot \rho u = 0, \\ &\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p = -\nabla \cdot \sigma, \\ &\partial_t E + \nabla \cdot (E + p) u = -\nabla \cdot q - \nabla \cdot (\sigma u), \end{aligned} \tag{15}$$

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

$$\sigma = -\mu \big(\nabla u + (\nabla u)^T - \frac{2}{3} \nabla \cdot u \big), \quad \text{and} \quad q = -\kappa \nabla \cdot T, \tag{16}$$

The viscosity and heat transfer coefficients are following:

$$\mu = \frac{\tau p}{2(1-\nu)}, \quad \text{and} \quad \kappa = \frac{5}{6} \tau p R. \tag{17}$$

The corresponding Prandtl number is $\mathrm{Pr} = \dfrac{3}{2(1-\nu)}$.

Complete ESFP model

Pros and cons

- \- We can only recover a Prandtl of 1 because ν is bounded below by $-\frac{1}{2}$ to ensure positiveness of the Θ tensor.
- \+ In real cases near equilibrium Θ is nearly equal to T**Id** so that we can use $\nu = -\frac{5}{4}$ and recover the correct Prandtl number.

Complete ESFP model

$$
\begin{aligned}
&\partial_t f + v \cdot \nabla_x f = D(f), \\
&D(f) = \frac{1}{\tau} \nabla_v \cdot \left((v - u) f + \Pi \nabla_v f \right), \\
&\Pi = (1 - \nu_{eff}) RTI + \nu_{eff} \Theta, \\
&\nu_{eff} = \max \left(-\frac{5}{4}, -\frac{RT}{\lambda_{max} - RT}) \right).
\end{aligned}
$$

Numerical method

Solving the collision operator

We use standard DSMC methods to proceed. Re-normalization is used to provide noiseless moments of the p.d.f. . One million particles are used.

Numerical test cases and solutions

- We present only 0-D test cases,
- Validation is made through two test cases, one with inactive correction on ν and one with active correction,
- One should recover the following ODEs for the Θ tensor and the third moment q.

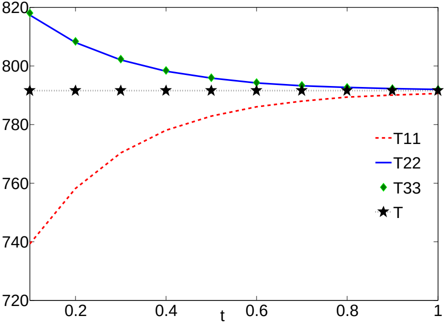
$$\frac{d}{dt}\Theta = \frac{1}{\tau}2(1-\nu)\left(RT-\Theta\right),$$

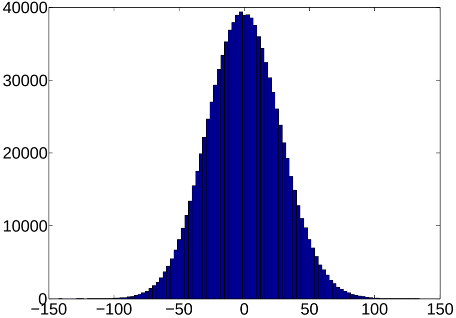
$$\Theta(t) = \exp\left(-\frac{2(1-\nu)t}{\tau}\right)\Theta(0) + \left(1-\exp\left(-\frac{2(1-\nu)t}{\tau}\right)\right)RTI,$$

(for ν constant)

$$\frac{d}{dt}q = -\frac{3}{\tau}q, \text{ so that } q(t) = q(0)\exp\left(-\frac{3t}{\tau}\right).$$

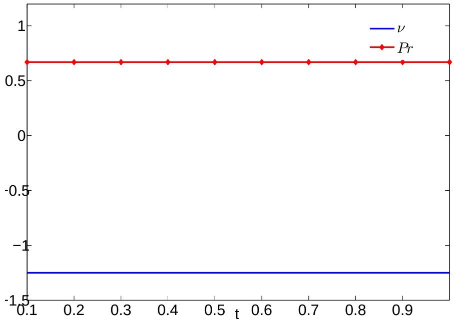
Numerical results for an homogeneous case: $\partial_t f = D(f)$ with inactive correction

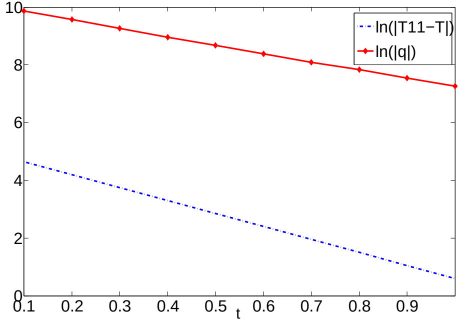




- On the left: behaviour of the diagonal components T_{11}, T_{22}, T_{33} of tensor Θ and of its trace T.
- On the right: histogram of the first component of velocity at time $t = 1$.

Numerical results for an homogeneous case: $\partial_t f = D(f)$ with inactive correction

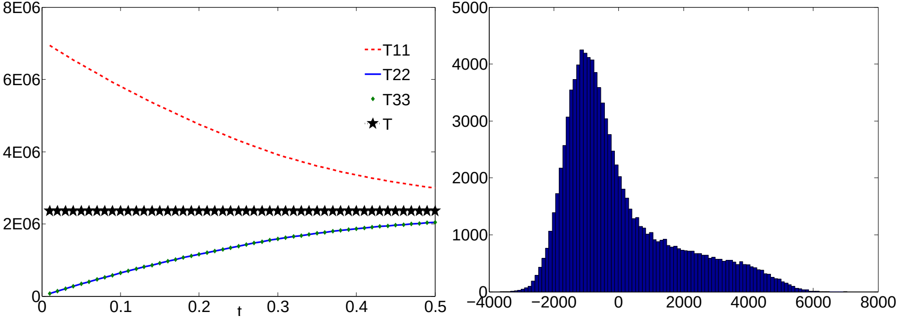




- On the left: ν and Pr along time.
- On the right: convergence of the logarithms of $|T - T_{11}|$ and q
- the Prandtl number numerically captured is equal to

$$Pr_n = \frac{2.8971}{4.5001} = 0.6428$$

Numerical results for an homogeneous case: $\partial_t f = D(f)$ with active correction



- On the left: behaviour of the diagonal components T_{11}, T_{22}, T_{33} of tensor Θ and of its trace T.
- On the right: histogram of the first component of velocity at time $t = 0.5$.

Numerical results for an homogeneous case: $\partial_t f = D(f)$ with active correction

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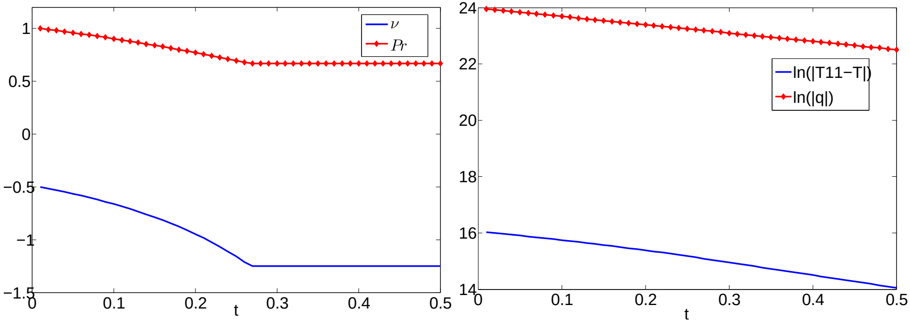
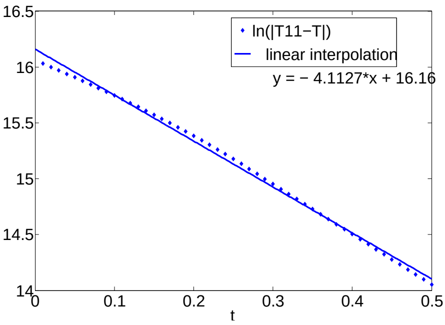
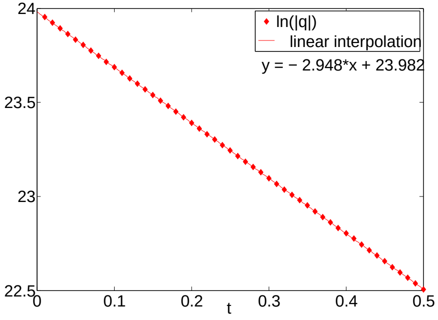


- On the left: ν and Pr along time.
- On the right: convergence of the logarithms of $|T - T_{11}|$ and q

Numerical results for an homogeneous case: $\partial_t f = D(f)$ with active correction



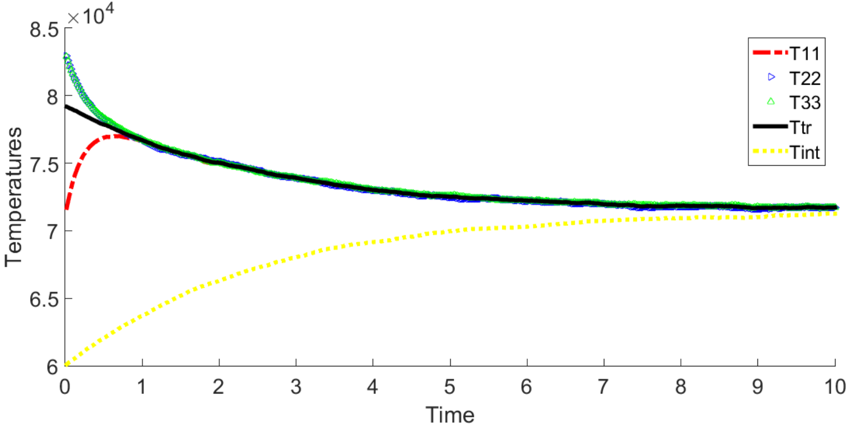


- On the left: comparison between $\log(|T - T_{11}|)$ ant its linear fitting.
- On the right: comparison between $\log(|q|)$ ant its linear fitting.

Conclusion & Perspectives

- Construction of a new kinetic model able to recover the correct Prandtl number in the hydrodynamic limit,
- More numerical tests need to be performed with a non homogeneous code,
- Extension to polyatomic gases necessary for real cases,
- Extension to chemistry / sprays should be investigated.

Numerical results for an homogeneous case: $\partial_t f = D(f)$ for polyatomic gases



- Convergence towards equilibrium for the different temperatures