Relaxation models of BGK type for gas mixtures
Part I

Marzia Bisi

Parma University, Italy

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Summary

First talk:

- Classical BGK relaxation model for a single species
- BGK model for an elastically scattering binary mixture

Second talk:

- Model of BGK type for a reacting mixture of four gases
- Possible generalizations and open problems
Kinetic description for a single gas

We consider a rarefied gas of particles with mass $m$ interacting through elastic collisions, preserving momentum and kinetic energy.

Distribution function: $f(t, x, \mathbf{v})$

Major macroscopic fields:

- number density: $n = \int f(\mathbf{v}) \, d\mathbf{v}$
- mean velocity: $\mathbf{u} = \frac{1}{n} \int \mathbf{v} f(\mathbf{v}) \, d\mathbf{v}$
- temperature: $T = \frac{m}{3nK} \int |\mathbf{v} - \mathbf{u}|^2 f(\mathbf{v}) \, d\mathbf{v}$
- viscous stress: $\mathbf{p} = m \int \left[ (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) - \frac{1}{3} |\mathbf{v} - \mathbf{u}|^2 \mathbf{I} \right] f(\mathbf{v}) \, d\mathbf{v}$
- heat flux: $\mathbf{q} = \frac{1}{2} m \int |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) f(\mathbf{v}) \, d\mathbf{v}$
\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = Q_{BE}(f, f)
\]
where
\[
Q_{BE}(f, f) = \int_{\mathbb{R}^3} \int_{S^2} |\mathbf{g}| \sigma(|\mathbf{g}|, \chi) \left[ f(\mathbf{v}')f(\mathbf{w}') - f(\mathbf{v})f(\mathbf{w}) \right] d\mathbf{w} d\hat{\Omega}'
\]
with
\((\mathbf{v}', \mathbf{w}')\) post–collision velocities corresponding to \((\mathbf{v}, \mathbf{w})\),
\(\mathbf{g} = \mathbf{v} - \mathbf{w} = |\mathbf{v} - \mathbf{w}| \hat{\Omega}\) relative velocity,
\(\sigma(|\mathbf{g}|, \chi)\) differential cross section depending on \(|\mathbf{g}|\) and on the
deflection angle \(\chi\)

**Remarks**

- The Boltzmann equation is of integro–differential type
- The analytical proofs and the numerical simulations strongly depend on the properties of the collision kernel \(|\mathbf{g}| \sigma(|\mathbf{g}|, \chi)\)
Motivation: to obtain simpler expressions for the collision term, able to reproduce essential features of the Boltzmann equation (collision invariants, Maxwellian equilibria, $H$–theorem)

References:

BGK kinetic equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = Q_{BGK} := \nu(M - f)$$

where
- $\nu$ is a collision frequency independent of molecular velocity $\mathbf{v}$
- $M$ is a suitable Maxwellian attractor $M = M(\tilde{n}, \tilde{u}, \tilde{T})$
\[ Q_{BGK} = \nu (M - f) \]
Here \( M \) is a local Maxwellian

\[ M = n \left( \frac{m}{2\pi KT} \right)^{3/2} \exp \left( - \frac{m}{2KT} |v - u|^2 \right) \]

with parameters \( n(t, x), u(t, x), T(t, x) \) coinciding with density, velocity, temperature of the gas, suitable integrals of the unknown distribution \( f \)

**Remark:**
In this operator, nonlinearity is hidden into the definition of \( n, u, T \)

**Properties:**

- **Collision invariants:**
  \[ \int \varphi(v) Q_{BGK}(f) \, dv = \nu \int \varphi(v) \left( M - f \right) \, dv = 0 \quad \varphi(v) = 1, \, v, \, |v|^2 \]

- **Collision equilibria:**
  \[ Q_{BGK}(f) = 0 \iff f = M, \] hence if \( f \) is a local Maxwellian
H-functional \textit{(in space homogeneous conditions)}:

$$H = \int f \log f \, dv$$

Entropy dissipation: $\dot{H} \leq 0, \forall f$, and equality holds only if $f = M$

Proof.

$$\dot{H} = \int \partial_t f \log f \, dv + \int \partial_t f \, dv = \nu \int (M - f) \log f \, dv$$

$$= \nu \int M \left(1 - \frac{f}{M}\right) \log \left(\frac{f}{M}\right) \, dv + \nu \int (M - f) \log M \, dv \leq 0$$

owing to convexity property of $(x - 1) \log x$ and to the fact that last integral vanishes since $\log M$ is a combination of collision invariants $1, v, |v|^2$
Collision frequency $\nu$

Remarks:
- All previous properties hold independently from the expression adopted for collision frequency $\nu$
- The quantity $\nu$ might take into account the intermolecular potential, namely the collision kernel of Boltzmann operator

Possible options to determine $\nu$:
1. We may impose that the BGK model preserves the exchange rate also for stress deviator:

$$m \int \left[ (v - u) \otimes (v - u) - \frac{1}{3} |v - u|^2 I \right] \left[ Q_{BGK}(f) - Q_{BE}(f, f) \right] dv = 0$$

2. We may equate BGK and Boltzmann averaged loss terms, in order to link $\nu$ to the actual number of collisions:

$$\nu = \frac{1}{n} \int \int \int |g| \sigma(|g|, \chi) f(v)f(w) dv dw d\hat{\Omega}$$

and these integrals (both in options 1) and 2)) may be explicitly evaluated for Maxwell molecules.
Possible generalizations of the classical BGK model

1. Models with $\nu$ depending on molecular velocity $v$ (useful for potentials in which collision frequency have strong variations for high molecular velocities)

2. Ellipsoidal BGK model:
   Motivation: Classical BGK does not reproduce the correct Prandtl number
   \[ \text{Pr} = \frac{5K\mu}{2m\kappa} \]
   \( \mu: \text{viscosity} \)
   \( \kappa: \text{conductivity} \)
   
   For Maxwell molecules $\text{Pr} = \frac{2}{3}$ since
   \[
   m \int \left[ (v-u) \otimes (v-u) - \frac{1}{3} |v-u|^2 I \right] Q_{BE}(f,f) \, dv = -\frac{3}{4} \nu_2 n p := -\alpha_p p \\
   \frac{1}{2} m \int |v-u|^2 (v-u) \, Q_{BE}(f,f) \, dv = -\frac{1}{2} \nu_2 n q := -\alpha_q q
   \]
   and $\text{Pr} = \alpha_q/\alpha_p$
Analogous computations show that the classical BGK operator
\[ Q_{BGK}(f) = \nu(M - f) \] provides \( Pr = 1 \)

**ES–BGK model:**


\[ Q_{ES-BGK}(f) = \nu(G - f) \] where

\[
G = n \frac{(\det A)^{1/2}}{\pi^{3/2}} \exp \left( - \sum_{i,j=1}^{3} A_{ij} (v_i - u_i)(v_j - u_j) \right)
\]

- If \( A = \frac{m}{2KT} I \), we recover classical BGK
- \( A = \left[ \frac{3KT}{m} I - \frac{1}{mn} p \right]^{-1} \) provides \( Pr = \frac{2}{3} \), and slight modifications of coefficients allow to reproduce also the Prandtl number corresponding to different intermolecular potentials
BGK models for mixtures - Some references

- Groppi, Monica, Spiga, *EPL* (2011)
- Bisi, Càceres, *(submitted)*
Boltzmann equations for gas mixtures

We consider now a gas of $N$ different elastically scattering species $G^s$, $s = 1, \ldots, N$

$\Rightarrow$ $N$ Boltzmann equations for distribution functions $f^s(t, x, v)$:

$$\frac{\partial f^s}{\partial t} + v \cdot \nabla_x f^s = Q_{BEel}^s = \sum_{r=1}^{N} Q_{el}^{sr}(f^s, f^r)$$

where

$$Q_{el}^{sr}(f^s, f^r) = \int_{\mathbb{R}^3} \int_{S^2} |g| \sigma^{sr}(|g|, \chi) \left[ f^s(v') f^r(w') - f^s(v) f^r(w) \right] dw d\hat{\Omega}'$$

takes into account the effects of elastic collisions between particles of species $(A^s, A^r)$

Collision equilibria: Maxwellian distributions with a common mean velocity and a common temperature ($N+4$ free parameters)

$$f_M^s = n^s \left( \frac{m^s}{2\pi K T} \right)^{3/2} \exp \left[ -\frac{m^s}{2K T} |v - u|^2 \right] \quad s = 1, \ldots, N$$
Remark: The trivial extension of the one–species BGK model

\[
\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_x f_s = \nu_s (M_s - f_s) \quad s = 1, \ldots, N
\]

with \( M_s \equiv M_s(n_s, \mathbf{u}^s, T^s) \) is obviously not consistent because it does not reproduce equilibrium conditions \( \mathbf{u}^s = \mathbf{u}, T^s = T, \forall s \)

**Pioneering models for mixtures:**
- Gross, Krook, Phys. Rev. (1956)
- Sirovich, Phys. Fluids (1962)
- McCormack, Phys. Fluids (1976)

\[
\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_x f_s = \sum_{r=1}^{N} \nu_{sr} (M_{sr} - f_s) \quad s = 1, \ldots, N
\]

with parameters of \( M_{sr} \) to be properly determined.

Unfortunately this model does not satisfy the **indifferentiability principle**: when all species are identical one does not recover the BGK equation for a single gas

A different model overcoming this drawback is proposed in Garzò, Santos, Brey, Phys. Fluids (1989), but positivity is lost
Consistent BGK model for mixtures


Model for an elastically scattering BINARY mixture:

\[
\begin{align*}
\frac{\partial f^1}{\partial t} + v \cdot \nabla_x f^1 &= \nu^1 (\mathcal{M}^1 - f^1) \\
\frac{\partial f^2}{\partial t} + v \cdot \nabla_x f^2 &= \nu^2 (\mathcal{M}^2 - f^2)
\end{align*}
\]

where \( \mathcal{M}^1 \equiv \mathcal{M}^1(n^1, \tilde{u}^1, \tilde{T}^1) \) and \( \mathcal{M}^1 \equiv \mathcal{M}^2(n^2, \tilde{u}^2, \tilde{T}^2) \)

\[
\mathcal{M}^s = n^s \left( \frac{m^s}{2\pi K \tilde{T}^s} \right)^{3/2} \exp \left( - \frac{m^s}{2K \tilde{T}^s} |v - \tilde{u}^s|^2 \right) \quad s = 1, 2
\]

\( \tilde{u}^1, \tilde{u}^2, \tilde{T}^1, \tilde{T}^2 \) are 8 auxiliary free parameters that have to be properly determined as functions of actual macroscopic parameters \( n^1, n^2, u^1, u^2, T^1, T^2 \) of the distribution functions \( f^1, f^2 \).
Auxiliary parameters \( \tilde{u}^1, \tilde{u}^2, \tilde{T}^1, \tilde{T}^2 \) are determined by imposing that Boltzmann (for Maxwell molecules) and BGK equations prescribe the same exchange rates for species mass velocities and temperatures:

\[
\int m^s v Q^s_{\text{BEel}} \, dv = \nu^s \int m^s v (M^s - f^s) \, dv \quad s = 1, 2
\]

\[
\frac{1}{2} \int m^s |v|^2 Q^s_{\text{BEel}} \, dv = \frac{1}{2} \nu^s \int m^s |v|^2 (M^s - f^s) \, dv \quad s = 1, 2
\]

For species 1 these constraints yield, respectively,

\[
\nu_1^{12} \mu^{12} n^1 n^2 (u^2 - u^1) = \nu^1 m^1 n^1 (\tilde{u}^1 - u^1)
\]

\[
\nu_1^{12} \frac{2 m^1 m^2}{(m^1 + m^2)^2} n^1 n^2 \left[ \frac{3}{2} K(T^2 - T^1) + \frac{1}{2} (m^1 u^1 + m^2 u^2) \cdot (u^2 - u^1) \right]
\]

\[
= \nu^1 \left[ \frac{3}{2} n^1 K(\tilde{T}^1 - T^1) + \frac{1}{2} m^1 n^1 (|\tilde{u}^1|^2 - |u^1|^2) \right]
\]

where \( \mu^{12} = \frac{m^1 m^2}{m^1 + m^2} \) and \( \nu_1^{12} \) is a (constant) microscopic collision frequency; analogous equalities hold for species 2.
By solving these equations we get

\[ \tilde{u}^1 = u^1 + \frac{\nu_1^{12}}{\nu_1} \frac{\mu^{12}}{m_1} n^2 (u^2 - u^1) \]

\[ \tilde{u}^2 = u^2 + \frac{\nu_1^{12}}{\nu_2} \frac{\mu^{12}}{m_2} n^1 (u^1 - u^2) \]

\[ K \tilde{T}^1 = KT^1 - \frac{2}{3} \frac{\nu_1^{12}}{\nu_1} \mu^{12} n^2 u^1 \cdot (u^2 - u^1) - \frac{1}{3m_1} \left( \frac{\nu_1^{12}}{\nu_1} \mu^{12} n^2 \right)^2 |u^2 - u^1|^2 \]

\[ + 2 \frac{\nu_1^{12}}{\nu_1} \frac{\mu^{12}}{m_1 + m_2} n^2 K(T^2 - T^1) + \frac{2}{3} \frac{\nu_1^{12}}{\nu_1} \frac{\mu^{12}}{m_1 + m_2} n^2 (m_1 u^1 + m_2 u^2) \cdot (u^2 - u^1) \]

and analogously (with exchanged indices) for \( \tilde{T}^2 \)
Collision invariants: imposing that BGK model preserves the exchange rates of Boltzmann equations for single $u^s$, $T^s$ gives consequently correct conservations of global velocity and of global temperature

$$u = \frac{m^1 n^1 u^1 + m^2 n^2 u^2}{m^1 n^1 + m^2 n^2}, \quad nKT = \sum_{s=1}^{2} \left[ n^s KT^s + \frac{1}{3} m^s n^s (|u^s|^2 - |u|^2) \right]$$

Collision equilibria:

$$Q^s_{BGK} = \nu^s (M^s - f^s) = 0 \quad \forall s$$ implies that equilibrium states are given by $f^s = M^s$, hence $u^s = \tilde{u}^s$ and $T^s = \tilde{T}^s$

By inserting these conditions into explicit expressions for $\tilde{u}^s$ and $\tilde{T}^s$ we get that Maxwellian equilibria are characterized by $u^1 = u^2 = u$ and $T^1 = T^2 = T$
Entropy dissipation:

\[ H = \sum_{s=1}^{2} \int f^s \log f^s \, dv \]

is a Lyapunov functional for the BGK model.

Sketch of the proof.

\[ \dot{H} = \sum_{s=1}^{2} \nu^s \int (M^s - f^s) \log f^s \, dv \]

Since \( U(y) = y \log y - y \) is convex and \( U'(y) = \log y \) we have

\[ (M^s - f^s) U'(f^s) = (M^s - f^s) \log f^s \leq U(M^s) - U(f^s) \]

de hence

\[ \dot{H} \leq \sum_{s=1}^{2} \nu^s \int \left( M^s \log M^s - f^s \log f^s \right) dv \]

\[ = \sum_{s=1}^{2} \nu^s \int \left( M^s \log M^s - f^s_M \log f^s_M \right) dv + \sum_{s=1}^{2} \nu^s \int \left( f^s_M \log f^s_M - f^s \log f^s \right) dv \]

where \( f^s_M = M^s(n^s, u^s, T^s) \) is the local equilibrium.
• The first term has the right sign ($\leq 0$) by direct computations, using explicit expressions for $\tilde{u}^s$ and $\tilde{T}^s$

• The second term is non–positive since

$$\int f_s^M \log f_s^M \, dv \leq \int f_s^s \log f_s^s \, dv \quad \forall s$$

(this is the $H$–theorem in the one species case)

Remark: Consistency of this BGK approximation holds also for an higher number of species, and this model has been generalized in Groppi, Spiga, Phys. Fluids (2004) to a chemically reacting mixture of four monoatomic gases

[Additional difficulties of the reactive frame: exchange rates are needed also for number densities, chemical exchange rates are explicit only under simplifying assumptions]
On the choice of $\nu^s$ and possible applications

**Numerical simulations** using such a BGK model:

- Comparison with deterministic kinetic calculations in space–homogeneous conditions  
- Study of classical space dependent problems, like steady shock–structure and Riemann problem  
- Semi–Lagrangian schemes for the whole (time and space dependent) BGK model  
  \((\text{Groppi, Puppo, Russo, Stracquadani (in preparation)})\)

\[ \Rightarrow \text{Collision frequencies are determined by equating the averaged loss term of BGK and Boltzmann equations (for Maxwell molecules)} \]

\[ \nu^s = \sum_{r=1}^{N} \nu_{sr}^0 n^r \]

with $\nu_{sr}^0$ suitable averages of the Boltzmann collision kernel  
\[ |g| \sigma^{sr}(|g, \chi|) = \nu^{sr}(\chi) \]
Damping forces and sound wave propagations in MEMS devices vibrating at high frequencies

(Bisi, Lorenzani, (2014, work in progress))

⇒ We use the linearized BGK equations \( f^s = f^s_M (1 + h^s) \), with \(|h^s| \ll 1\), and collision frequencies are determined by equating exchange rates of BGK and Boltzmann equations for viscous stress tensors

\[
\nu^1 = \frac{3}{4} \nu_2^{11} n^1_M + \frac{3}{2} \nu_2^{12} \frac{\mu^{12}}{m^1} n^2_M \quad \nu^2 = \frac{3}{2} \nu_2^{12} \frac{\mu^{12}}{m^2} n^1_M + \frac{3}{4} \nu_2^{22} n^2_M
\]

Forthcoming talk:

- A (different) BGK model for chemically reacting mixtures
- Generalization to mixtures of polyatomic gases
Thank you for your attention