Relaxation models of BGK type for gas mixtures
Part II

Marzia Bisi

Parma University, Italy

7th edition of the Summer School on
METHODS AND MODELS OF KINETIC THEORY
Porto Ercole (Grosseto), June 8–14, 2014
Summary

- BGK relaxation model for a reacting mixture of four gases  
  (*Bisi, Groppi, Spiga, Proceedings RGD26 (2009)*)

- Generalization to a mixture of polyatomic gases  
  (*Bisi, Caceres, submitted (2014)*)

- Future works and open problems
Kinetic approach to chemically reacting mixtures


Physical frame:

- Mixture of four gases $G^s$ $\ s = 1, \ldots, 4$
- Each particle of the gas $G^s$ is characterized by its own molecular velocity $v$ and by an internal energy $E^s$
- Besides elastic collisions, particles are subject to the bimolecular and reversible chemical reaction

\[ G^1 + G^2 \leftrightarrow G^3 + G^4 \]

- Conservation of mass implies $m^1 + m^2 = m^3 + m^4$
- Direct reaction is assumed endothermic:

\[ \Delta E = E^3 + E^4 - E^1 - E^2 > 0 \]
Boltzmann equations

\[ \frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_x f_s = Q_{BEel}^s(f) + Q_{BEch}^s(f) \quad s = 1, 2, 3, 4 \]

where \( Q_{BEel}^s \) is the elastic collision operator and \( Q_{BEch}^s \) is the chemical collision operator.

\[ Q_{BEch}^1 = \int_{\mathbb{R}^3} \int_{S^2} U \left( |\mathbf{g}|^2 - \frac{2 \Delta E}{\mu_{12}} \right) |\mathbf{g}| \sigma_{34}^{12}(|\mathbf{g}|, \chi) \left[ \left( \frac{\mu_{12}^3}{\mu_{34}^3} \right) f^3(\mathbf{v}') f^4(\mathbf{w}') - f^1(\mathbf{v}) f^2(\mathbf{w}) \right] d\mathbf{w} d\hat{\Omega}' \]

- Chemical operators for other species may be obtained by suitable permutations of indices.
- \( U \) stands for a unit step function, and it represents a threshold for the endothermic reaction.
- The ratio \( (\mu_{12} / \mu_{34})^3 \) is due to the Jacobian of the change of variables pre- ↔ post–collision velocities.
- Differential cross section of direct and reverse reaction are related by the microreversibility condition.
Collision equilibria:

\[ f_s^M = n_s \left( \frac{m_s}{2\pi KT} \right)^{3/2} \exp \left[ -\frac{m_s}{2KT} |v - u|^2 \right] \quad s = 1, \ldots, 4 \]

+ mass action law:

\[ \frac{n_1 n_2}{n_3 n_4} = \left( \frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \exp \left( \frac{\Delta E}{KT} \right) \]

\[ H-\text{functional:} \quad H = \sum_{s=1}^{4} \int f^s(v) \log \left( \frac{f^s(v)}{(m_s^s)^3} \right) dv \]

Conservation laws:

- \( n^1 + n^3, \quad n^1 + n^4, \quad n^2 + n^4 \)
  combinations of number densities

- \( u \)  global momentum

- \( \frac{3}{2} nKT + \sum_{s=1}^{4} E^s n^s \)  total (kinetic + chemical) energy
Reactive BGK relaxation model

(Bisi, Groppi, Spiga (2009))

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

where

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

Differences with respect to the inert BGK model by Andries, Aoki, Perthame (2002):

- auxiliary number densities $\tilde{n}^s$ are different from the actual ones;
- Maxwellian attractors are accommodated at a common mean velocity $\tilde{u}$ and temperature $\tilde{T}$

$\Rightarrow$ In this model we have 8 free auxiliary parameters $\tilde{n}^s$, $\tilde{u}$, $\tilde{T}$ to be determined in terms of the actual macroscopic fields
Auxiliary parameters

\( \tilde{n}^s, \tilde{u}, \tilde{T} \), are bound together by the mass action law

\[
\frac{\tilde{n}^1 \tilde{n}^2}{\tilde{n}^3 \tilde{n}^4} = \left( \frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \exp \left( \frac{\Delta E}{K \tilde{T}} \right)
\]

and by imposing that reactive Boltzmann and BGK equations prescribe the same collision invariants

\[
\int (Q_{BGK}^s + Q_{BGK}^r) \, dv = 0 \quad (s, r) = (1, 3), (1, 4), (2, 4),
\]

\[
\sum_{s=1}^{4} \int m^s v Q_{BGK}^s \, dv = 0, \quad \sum_{s=1}^{4} \int \left( \frac{1}{2} m^s v^2 + E^s \right) Q_{BGK}^s \, dv = 0
\]

⇒ These are exactly eight constraints for the eight auxiliary parameters of the BGK model
Collision invariants provide seven independent algebraic equations that allow to express parameters $\tilde{n}_2, \tilde{n}_3, \tilde{n}_4, \tilde{u}, \tilde{T}$ in terms of $\tilde{n}_1$ and of the actual fields $n^s, u^s, T^s$:

$$\tilde{n}^s = n^s + \lambda^s \nu^1 \nu^s (\tilde{n}_1 - n^1), \quad s = 2, 3, 4, \quad \lambda^1 = \lambda^2 = -\lambda^3 = -\lambda^4 = 1$$

$$\tilde{u} = \sum_{s=1}^{4} \nu^s m^s n^s u^s / \sum_{s=1}^{4} \nu^s m^s n^s$$

$$\tilde{T} = \left\{ \sum_{s=1}^{4} \nu^s n^s \left[ \frac{1}{2} m^s ((u^s)^2 - \tilde{u}^2) + \frac{3}{2} K T^s \right] + \nu^1 \Delta E (\tilde{n}_1 - n^1) \right\} \frac{1}{\frac{3}{2} K \sum_s \nu^s n^s}$$

$\tilde{n}_1$ is determined by the mass action law:

$$F(\tilde{n}_1) = \left( \frac{m^1 m^2}{m^3 m^4} \right)^{3/2} \text{ where } F(\tilde{n}_1) = \frac{\tilde{n}_1 \tilde{n}_2 (\tilde{n}_1)}{\tilde{n}_3(\tilde{n}_1) \tilde{n}_4(\tilde{n}_1)} \exp \left( - \frac{\Delta E}{K \tilde{T}(\tilde{n}_1)} \right)$$

This is a transcendental equation for $\tilde{n}_1$. It may be proved that:

- $F$ is a monotonically increasing function of its argument
- $F$ varies from 0 to $+\infty$ for $\tilde{n}_1$ ranging in the interval allowed to ensure positivity of all $\tilde{n}^s$ and of $\tilde{T}$

$\Rightarrow$ there exists a unique physically admissible value for $\tilde{n}_1$
Properties

1. **Conservation equations**: they are guaranteed by the method of construction of this BGK model

   \[\text{[With respect to the model by Groppi, Spiga (2004), here we lose the preservation of exchange rates of single species velocities and temperatures]}\]

2. **Collision equilibria**:

   \[f^s(v) = M^s(v) \quad \forall v \in \mathbb{R}^3 \quad \Rightarrow \quad n^s = \tilde{n}^s, \quad u^s = \tilde{u}, \quad T^s = \tilde{T}\]

   hence also the actual parameters are related by the mass action law

3. **$H$–functional**:

   \[H = \sum_{s=1}^{4} \int f^s \log \frac{f^s}{(m^s)^3} \, dv\]

   is a Lyapunov functional for the space homogeneous BGK model
Entropy dissipation: \[ \dot{H} = \sum_{s=1}^{4} \int Q_{BGK}^s \log \frac{f^s}{(m^s)^3} \, dv \leq 0 \]

Proof.

\[ \sum_{s=1}^{4} \int Q_{BGK}^s \log \frac{M^s}{(m^s)^3} \, dv \]
\[ = \sum_{s=1}^{4} \nu^s \int (M^s - f^s) \left[ \log \frac{\tilde{n}^s}{(m^s)^{3/2}} - \frac{3}{2} \log(2\pi K \tilde{T}) - \frac{m^s}{2K \tilde{T}} |v - \tilde{u}|^2 \right] \, dv \]
\[ = \nu^1 (\tilde{n}^1 - n^1) \left\{ \log \left[ \frac{\tilde{n}^1 \tilde{n}^2}{\tilde{n}^3 \tilde{n}^4} \left( \frac{m^3 m^4}{m^1 m^2} \right)^{3/2} \right] - \frac{\Delta E}{K \tilde{T}} \right\} = 0 \]

owing to conservation laws and to mass action law for auxiliary parameters

\[ \Rightarrow \dot{H} = - \sum_{s=1}^{4} \nu^s \int (f^s - M^s) \log \frac{f^s}{M^s} \, dv \leq 0 \]
Hydrodynamic regime
(Bisi, Groppi, Spiga, Phys. Rev. E (2010))

\[
\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \nabla_x f^s = \frac{1}{\varepsilon} \nu^s (\mathcal{M}^s - f^s) \quad s = 1, \ldots, 4
\]

Chapman–Enskog asymptotic expansion: \( f^s = f^{s(0)} + \varepsilon f^{s(1)} \)
and consequently similar expansions hold for \( n^s, u^s, T^s \), leaving hydrodynamic variables unexpanded

- **Leading order accuracy:**

  \[
  f^{s(0)} = \mathcal{M}^{s(0)} \quad \Rightarrow \quad f^{s(0)}(\mathbf{v}) = n^{s(0)} \left( \frac{m^s}{2\pi K T^{(0)}} \right)^{\frac{3}{2}} \exp \left[ -\frac{m^s}{2 K T^{(0)}} |\mathbf{v} - \mathbf{u}|^2 \right]
  \]

  with \( n^{s(0)} \) and \( T^{(0)} \) bound together by the mass action law

- **First–order correction:**

  \[
  \nu^{s(0)} \left[ \mathcal{M}^{s(1)}(\mathbf{v}) - f^{s(1)}(\mathbf{v}) \right] = \frac{\partial_0 f^{s(0)}}{\partial t} + \mathbf{v} \cdot \nabla_x f^{s(0)}
  \]
Standard manipulations allow to obtain an explicit expression for \( f^{s(1)} \)

- Onsager relations for species mass velocities:

\[
\mathbf{u}^{s(1)} = - \sum_{r=1}^{4} L^{sr(0)} \frac{1}{\rho^{s(0)} \rho^{r(0)}} \nabla_x (n^{r(0)} KT^{(0)})
\]

- Additional scalar pressure:

\[
T^{(1)} = - \frac{2}{3} KT^{(0)} \left[ \frac{1}{n} \sum_{s=1}^{4} \frac{n^{s(0)}}{\nu^{(0)}_s} + \frac{3}{2} n \left( \frac{KT^{(0)}}{\Delta E} \right)^2 \sum_{s=1}^{4} \frac{1}{\nu^{(0)}_s n^{s(0)}} \right] \nabla_x \cdot \mathbf{u}
\]

- Viscous stress and heat flux formally coincide with those relevant to an inert mixture and, as expected, they provide \( \text{Pr} = 1 \)
Chu decomposition of the distribution functions for axially symmetric problems (with respect to $x_1 = x$)

\[
\phi^s = \int \int f^s \, dv_2 \, dv_3 \quad \psi^s = \int \int (v_2^2 + v_3^2) f^s \, dv_2 \, dv_3
\]

\[
\Rightarrow \quad \frac{\partial \phi^s}{\partial t} = \nu^s (\tilde{M}^s - \phi^s) \quad \frac{\partial \psi^s}{\partial t} = \nu^s \left( \frac{2K\tilde{T} m^s}{m^s} \tilde{M}^s - \psi^s \right)
\]

This system is simulated by a Runge-Kutta explicit method

Macroscopic moments are reconstructed as

\[
n^s = \int \phi^s \, dv, \quad u^s = \frac{1}{n^s} \int v \phi^s \, dv,
\]

\[
\frac{3K T^s}{m^s} = \frac{1}{n^s} \left[ \int |v - u^s|^2 \phi^s \, dv + \int \psi^s \, dv \right]
\]
Relaxation parameters $\nu^s$
related to the actual number of collisions undergone in a unit time

- **Elastic collision frequencies**: for Maxwellian molecules, the loss term for species $s$ scattering with species $r$ is $-\nu^{sr}_0 n^r f^s$

  \[
  \Rightarrow \quad \nu_{\text{mech}}^s = \sum_{r=1}^{4} \nu^{sr}_0 n^r \quad s = 1, \ldots, 4
  \]

- **Chemical collision frequencies**: we assume Maxwell–like collision model for the exothermic reaction with activation energy $A \geq 0$

  \[
  \nu_{\text{chem}}^3 = \nu_{34}^{12} \frac{1}{n^3} \iiint \Theta \left( |g|^2 - \frac{2A}{\mu^{34}} \right) f^3(v) f^4(w) \, dv \, dw
  \]

  \[
  \nu_{\text{chem}}^1 = \frac{1}{n^1} \iiint \sigma_{12}^{34}(|g|, \chi) f^1(v) f^2(w) \, dv \, dw \, d\hat{\Omega}'
  \]

- In conclusion, $\nu^s = \nu_{\text{mech}}^s + \nu_{\text{chem}}^s$ and chemical integrals may be explicitly solved by approximating all distribution functions $f^s$ by local Maxwellians
Initial distributions are **Maxwellian shapes** characterized by

\[ m^1 = 11.7 \quad m^2 = 3.6 \quad m^3 = 8 \quad m^4 = 7.3 \]

\[ E^1 = 3 \quad E^2 = 2 \quad E^3 = 4 \quad E^4 = 7 \quad \Rightarrow \Delta E = 6 \]

\[ n_0^1 = 11 \quad n_0^2 = 9 \quad n_0^3 = 10 \quad n_0^4 = 7 \]

\[ u_0^1 = 1 \quad u_0^2 = -2 \quad u_0^3 = 3 \quad u_0^4 = -5.94 \quad \Rightarrow \quad u_0 = 0 \]

\[ T_0^1 = 8 \quad T_0^2 = 5 \quad T_0^3 = 7 \quad T_0^4 = 6 \quad \Rightarrow \quad T_0 = 31.7175 \]

\[ \Rightarrow \quad \text{Corresponding (uniquely determined) equilibrium values:} \]

\[ n_M^1 = 9.536, \quad n_M^2 = 7.536, \quad n_M^3 = 11.464, \quad n_M^4 = 8.464, \quad T_M = 31.559 \]

**Collision frequencies:**

<table>
<thead>
<tr>
<th>( \nu_{0}^{sr} )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>( \nu_{34}^{12} ) = 0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.3</td>
<td>0.4</td>
<td>0.1</td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.4</td>
<td>0.3</td>
<td>0.4</td>
<td>0.6</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>0.4</td>
<td>0.3</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.4</td>
<td>0.6</td>
<td>0.2</td>
<td>0.4</td>
<td></td>
</tr>
</tbody>
</table>
Actual (solid lines) and auxiliary (dash-dot lines) number densities (left) and global temperature (right)
Time evolution of $\phi^s$
Variation: initial distributions given by sums of two Gaussians, symmetric with respect to $u^s$, chosen in such a way that initial macroscopic moments remain the same as in the reference case.
Kinetic approach to polyatomic gases:
each gas is endowed with a suitable internal energy variable to mimic non–translational degrees of freedom

- **Groppi, Spiga, J. Math. Chem. (1999):** discrete internal energy levels;
- **Desvillettes, Monaco, Salvarani, Europ. J. Mech. B/Fluids (2005):** continuous internal energy variable

Our physical frame:
- mixture of four gases $G^1, G^2, G^3, G^4$
- each gas $G^s$ is considered as a mixture of $Q$ monoatomic components $A^i, \ i = s, \ s + 4, \ s + 8, \ s + 4(Q - 1)$, each one characterized by a different internal energy $E^i$
- in the frame of each species, energies are monotonically increasing with their index:

$$\forall \ i, j \equiv s, \ i < j \ \Rightarrow \ E^i < E^j$$
Besides elastic scattering and chemical reactions

\[ A^i + A^j \rightleftharpoons A^h + A^k \quad i \equiv 1, \quad j \equiv 2, \quad h \equiv 3, \quad k \equiv 4 \]

particles may undergo also inelastic transitions

\[ A^i + A^j \rightleftharpoons A^h + A^k \quad h \equiv i, \quad k \equiv j \]

Collision invariants:

\[ N^1 + N^3, \quad N^1 + N^4, \quad N^2 + N^4 \quad \text{where} \quad N^s = \sum_{i=s} n^i, \]

global velocity \( u \),

global energy \( \frac{3}{2} nKT + \sum_{i=1}^{4Q} E^i n^i \)
Collision equilibria of the Boltzmann equations:

\[ f_i^i(M(v)) = n_i \left( \frac{m_s}{2\pi KT} \right)^{3/2} \exp \left[ -\frac{m_s}{2KT}|v-u|^2 \right] \quad \forall i \equiv s, \quad \forall s = 1, \ldots, 4, \]

with equilibrium number densities related by the constraints

\[ n_i = N^s \psi(E^i, T) \]

where

\[ \psi(E^i, T) = \frac{\exp \left( -\frac{E^i-E^s}{KT} \right)}{\sum_{i \equiv s} \exp \left( -\frac{E^i-E^s}{KT} \right)} = \frac{\exp \left( -\frac{E^i-E^s}{KT} \right)}{Z^s(T)}, \]

and by the mass action law of chemistry

\[ \frac{N^1 N^2}{N^3 N^4} = \left( \frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \frac{Z^1(T)Z^2(T)}{Z^3(T)Z^4(T)} e^{\frac{\Delta E^{34}_{12}}{KT}} \]

where \( \Delta E^{34}_{12} = E^3 + E^4 - E^1 - E^2 > 0 \)

Remark: \( \psi(E^i, T) \) represents the fraction of particles \( G^s (s \equiv i) \) belonging to the component \( A^i \) in any equilibrium configuration; for any \( i, j \) with \( i \equiv j \) and \( i < j \), we have \( \psi(E^i, T) > \psi(E^j, T) \)
\[
\frac{\partial f^i}{\partial t} + \mathbf{v} \cdot \nabla_x f^i = \nu^i (\mathcal{M}^i - f^i) \quad i = 1, \ldots, 4Q
\]

where attractors \( \mathcal{M}^i \) take the form

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

while fictitious densities \( \tilde{n}^i \) are taken bound together as

\[
\tilde{n}^i = \tilde{N}^s \psi(\mathbf{E}^i, \tilde{T}), \quad \frac{\tilde{N}^1 \tilde{N}^2}{\tilde{N}^3 \tilde{N}^4} = \left( \frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \frac{Z^1(\tilde{T}) Z^2(\tilde{T})}{Z^3(\tilde{T}) Z^4(\tilde{T})} e^{\frac{\Delta E_{12}^{34}}{kT}} \tag{a}
\]

\( \Rightarrow \) 7 independent free parameters (\( \tilde{u} \), \( \tilde{T} \), three among \( \tilde{N}^s \)) to be determined imposing the preservation of correct collision invariants
\[
\sum_{i \equiv s} v^i \int (M^i - f^i) d\mathbf{v} + \sum_{i \equiv r} v^i \int (M^i - f^i) d\mathbf{v} = 0
\]
\[
(s, r) = (1, 3), (1, 4), (2, 4)
\]  
\[\text{(b)}\]

\[
\sum_{s=1}^{4} \sum_{i \equiv s} v^i \int m^s v (M^i - f^i) d\mathbf{v} = 0
\]  
\[\text{(c)}\]

\[
\sum_{s=1}^{4} \sum_{i \equiv s} v^i \int \left(\frac{1}{2} m^s |\mathbf{v}|^2 + E^i\right) (M^i - f^i) d\mathbf{v} = 0
\]  
\[\text{(d)}\]

- Conditions (b) allow to express three among the auxiliary number densities (i.e. \(\tilde{N}^2, \tilde{N}^3, \tilde{N}^4\)) in terms of the fourth one (\(\tilde{N}^1\)), the auxiliary temperature \(\tilde{T}\) and the actual number densities \(n^i\)

\[
\frac{\tilde{N}^s}{Z^s(\tilde{T})} = \frac{1}{\sum_{i \equiv s} v^i e^{-\frac{E^i-E^s}{kT}}} \left\{ \sum_{i \equiv s} v^i n^i - \lambda^s \sum_{i \equiv 1} v^i n^i + \lambda^s \left( \sum_{i \equiv 1} v^i e^{-\frac{E^i-E^1}{kT}} \right) \frac{\tilde{N}^1}{Z^1(\tilde{T})} \right\}
\]

\[(s = 2, 3, 4) \text{ where } \lambda^1 = \lambda^2 = 1, \lambda^3 = \lambda^4 = -1\]
Condition (c) yields

\[ \tilde{u} = \left( \sum_{s=1}^{4} m^s \sum_{i=s}^{\nu^i n^i u^i} \right) \left/ \left( \sum_{s=1}^{4} m^s \sum_{i=s}^{\nu^i n^i} \right) \right. \]

Energy conservation (d) provides

\[ \frac{3}{2} \left( \sum_{i=1}^{4Q} \nu^i n^i \right) K \tilde{T} + \sum_{s=1}^{4} \frac{\tilde{N}^s}{Z^s(\tilde{T})} \sum_{i=s}^{\nu^i E^i \ e^{- \frac{E^i - E^s}{kT}}} = \Lambda \quad \text{(d\*)} \]

where \( \Lambda \) is a known explicit function of the actual parameters

**Main difference** with respect to the monoatomic mixture: (d\*) and mass action law (a) are two transcendental equations for the unknowns (\( \tilde{N}^1, \tilde{T} \))
• By inserting into $(d^*)$ the explicit expressions of $\tilde{N}^2$, $\tilde{N}^3$, $\tilde{N}^4$, it becomes a “linear” equation for $\tilde{N}^1$, providing

$$\tilde{N}^1 = \frac{Z^1(\tilde{T})}{\sum_{i=1} \nu_i e^{-\frac{E_i-E_1}{kT}}} \left[ \sum_{i=1} \nu_i n^i + S(\tilde{T}) \right] \text{ where } S(\tilde{T}) = \frac{N(\tilde{T})}{D(\tilde{T})}$$

(with $N(\tilde{T})$ and $D(\tilde{T})$ complicated but explicit functions of the unknown $\tilde{T}$)

• With some manipulations, mass action law (a) may be cast as

$$G(\tilde{T}) = \left( \frac{\mu_{12}}{\mu_{34}} \right)^{3/2}$$

where

$$G(\tilde{T}) = \frac{\left[ \sum_{i=1} \nu_i n^i + S(\tilde{T}) \right] \left[ \sum_{j=2} \nu_j n^j + S(\tilde{T}) \right]}{\sum_{h=3} \nu_h n^h - S(\tilde{T}) \left[ \sum_{k=4} \nu_k n^k - S(\tilde{T}) \right]} \sum_{h=3} \nu_h e^{-\frac{E_h-E_3}{kT}} \sum_{k=4} \nu_k e^{-\frac{E_k-E_4}{kT}} e^{-\frac{\Delta E_{12}}{kT}}$$

(the contents of the square brackets are essentially the number densities)
We must prove that equation \( G(\tilde{T}) = \left( \frac{\mu_{12}}{\mu_{34}} \right)^{3/2} \) admits a positive solution in the range for which all densities are positive, hence in the set

\[
A = \left\{ \tilde{T} > 0 : \max \left( - \sum_{i=1}^{\nu} n_i^i, - \sum_{i=2}^{\nu} n_i^i \right) < S(\tilde{T}) < \min \left( \sum_{i=3}^{\nu} n_i^i, \sum_{i=4}^{\nu} n_i^i \right) \right\}
\]

**Steps of the proof:**

- we prove that in any interval \((\tilde{T}_1, \tilde{T}_2) \subseteq A\) in which the sign of the denominator \(D(\tilde{T})\) does not change, the function \(S(\tilde{T}) = N/D\) is strictly monotone; more precisely, \(S(\tilde{T})\) is increasing if \(D(\tilde{T}) < 0\), and \(S(\tilde{T})\) is decreasing if \(D(\tilde{T}) > 0\);

- we actually notice that \(A\) is a connected set of \(\mathbb{R}^+\) and the sign of \(D(\tilde{T})\) does not change in \(A\);

- we prove that \(G(\tilde{T})\) is strictly monotone in \(A\) and it ranges from 0 to \(+\infty\), providing does a unique solution to our equation

\[\Rightarrow\] The proposed BGK model for polyatomic reacting gas mixtures is well defined, and it may be proved that correct collision equilibria and \(H\)–theorem are reproduced
Open problems

- Ellipsoidal BGK models for (polyatomic) gas mixtures
  - Groppi, Monica, Spiga, EPL (2011) - for an inert binary mixture
  - Brull, Schneider, Commun. Math. Sci. (in press, 2014) - for a mixture of monoatomic gases

- Entropy dissipation estimates
  If we denote the relative entropy as
  \[ H(f | f_M) = \sum_{s=1}^{4} \int f^s \log \left( \frac{f^s}{f_M^s} \right) dv \]
  we have
  \[ \dot{H}(f | f_M) = - D(f) \leq 0 \]
  and we would like to prove a functional inequality of the form
  \[ D(f) \geq \lambda \Phi(H(f | f_M)) \]
  for some \( \lambda > 0 \) and for some non-decreasing continuous function \( \Phi \)
Thank you for your attention