Shock structure for macroscopic multi-temperature model of binary mixtures: comparison with kinetic models

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Problems on
Kinetic theory and PDE’s,
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Motivation

1. Shock structure analysis in rarefied gas mixture

2. Multi-temperature hyperbolic model of binary mixtures

3. Validating the existence of the temperature overshoot of the heavier component (Argon) within the simplicity of the model

4. Comparison with kinetic theory results
Outline

Introduction

Model

Comparison with experimental results

Systematic analysis and results
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Why multi-temperature?

1. **Kinetic theory** → nonequal partition of internal energy

2. **Plasma physics:**

   \[ T_e \gg T_i \]

3. **Mixture of gases with different molecular masses:**

   \[ m_1 < m_2, \quad \mu = \frac{m_1}{m_2}, \quad m_{He} < m_{Ar}, \quad \Rightarrow \quad T_{He} \neq T_{Ar} \]
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Governing equations:

Balance laws for mass, momentum and energy:

\[
\frac{\partial \rho_\alpha}{\partial t} + \text{div}(\rho_\alpha \mathbf{v}_\alpha) = \tau_\alpha, \quad \text{inert gases} \Rightarrow \tau_\alpha = 0,
\]

\[
\frac{\partial (\rho_\alpha \mathbf{v}_\alpha)}{\partial t} + \text{div}(\rho_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha - \mathbf{t}_\alpha) = \mathbf{m}_\alpha,
\]

\[
\frac{\partial \left( \frac{1}{2} \rho_\alpha \mathbf{v}_\alpha^2 + \rho_\alpha \varepsilon_\alpha \right)}{\partial t} + \text{div} \left\{ \left( \frac{1}{2} \rho_\alpha \mathbf{v}_\alpha^2 + \rho_\alpha \varepsilon_\alpha \right) \mathbf{v}_\alpha - \mathbf{t}_\alpha \mathbf{v}_\alpha + \mathbf{q}_\alpha \right\} = \mathbf{e}_\alpha,
\]

Trusdell principles → all quantities have to be conserved:

\[
\sum_\alpha \tau_\alpha = 0; \quad \sum_\alpha \mathbf{m}_\alpha = 0; \quad \sum_\alpha \mathbf{e}_\alpha = 0;
\]
Global field variables

Link with properties of the mixture components:

\[ c = \frac{\rho_1}{\rho}, \quad \rho = \sum_{\alpha=1}^{2} \rho_\alpha, \quad v = -\frac{1}{\rho} \sum_{\alpha=1}^{2} \rho_\alpha v_\alpha, \quad u_\alpha = v_\alpha - v, \]

\[ \varepsilon_1 = \frac{1}{\rho} \sum_{\alpha=1}^{2} \rho_\alpha \varepsilon_\alpha, \quad \varepsilon = \varepsilon_1 + \frac{1}{2\rho} \sum_{\alpha=1}^{2} \rho_\alpha u_\alpha^2, \quad p = \sum_{\alpha=1}^{2} p_\alpha, \]

\[ t = \sum_{\alpha=1}^{2} (t_\alpha - \rho_\alpha u_\alpha \otimes u_\alpha), \quad q = \sum_{\alpha=1}^{2} \left\{ q_\alpha + \rho_\alpha \left( \varepsilon_\alpha + \frac{1}{2} u_\alpha^2 \right) u_\alpha - t_\alpha u_\alpha \right\} \]

Non-equilibrium variables:

1. Diffusion flux vector: \( J = \rho_1 u_1 = -\rho_2 u_2 \)
2. Diffusion temperature: \( \Theta = T_2 - T_1 \)
Basic assumptions (1)

1. State variables $\rightarrow \rho_\alpha, v_\alpha, T_\alpha$

2. Constitutive relations $\rightarrow$ components are ideal gases $\rightarrow$ classic thermal and caloric equations of state:

$$p_\alpha = \rho_\alpha \frac{k_B}{m_\alpha} T_\alpha, \quad \varepsilon_\alpha = \frac{k_B}{m_\alpha} \frac{T_\alpha}{\gamma_\alpha - 1}.$$

a) Inviscid approximation $\rightarrow$ nor viscous nor neat conducting:

$$t_\alpha = -p_\alpha I, \quad q_\alpha = 0 \quad (\alpha = 1, 2).$$
Basic assumptions (2)

b) Viscous approximation $\rightarrow$ classic constitutive relations of Navier-Stokes-Fourier type:

\[ t_\alpha = -p_\alpha I + \sigma_\alpha, \quad \sigma_\alpha = 2\mu_\alpha D_\alpha, \]

\[ D_\alpha = \frac{1}{2} \left( \nabla v_\alpha + (\nabla v_\alpha)^T \right), \]

\[ q_\alpha = -\kappa_\alpha \nabla T_\alpha, \quad (\alpha = 1, 2) \]

c) Kinetic theory $\rightarrow$

Hard spheres model $\rightarrow$ viscosity and heat conductivity

\[ \mu_{10} = \frac{5}{16} \frac{a_0}{\sqrt{\pi} d_1^2} \sqrt{\frac{m_0 m_1}{\gamma}}, \quad \mu_{20} = \frac{5}{16} \frac{a_0}{\sqrt{\pi} d_2^2} \sqrt{\frac{m_0 m_2}{\gamma}}, \]

\[ \kappa_{10} = \frac{15}{4} \frac{k_B}{m_1} \mu_{10}, \quad \kappa_{20} = \frac{15}{4} \frac{k_B}{m_2} \mu_{20}, \]
Average temperature of the mixture

**Temperature** → average molecular kinetic energy.

\[
\rho \varepsilon_I = \sum_{\alpha=1}^{n} \rho_\alpha \varepsilon_\alpha(\rho_\alpha, T_\alpha)
\]

\[
(\rho_1 c_{V_1} + \rho_2 c_{V_2}) T = \rho_1 c_{V_1} T_1 + \rho_2 c_{V_2} T_2, \quad \varepsilon_I = \frac{k_B}{m} \frac{T}{\gamma - 1} = \frac{3}{2} \frac{k_B}{m} T
\]

\[
T = c \frac{m}{m_1} T_1 + (1 - c) \frac{m}{m_2} T_2
\]

\[
T_1 = T - \frac{(1 - c) \mu}{c + (1 - c) \mu} \Theta, \quad T_2 = T + \frac{c}{c + (1 - c) \mu} \Theta
\]

T. Ruggeri and S. Simic, Average temperature and maxwellian iteration in multitemperature mixtures of fluids, Phys. Rev. E 80 (2009), 026317. 9 of 31
Structure of source terms (1)

Basic principles of extended termodynamics:

• Galelian invariance:

\[ m_1 = \hat{m}_1 = -m_2, \quad e_1 = \hat{e}_1 + \hat{m}_1 \cdot v = -e_2, \]

• Entropy principle:

\[ \hat{m}_1 = -\psi_{11} \left( \frac{u_1}{T_1} - \frac{u_2}{T_2} \right), \quad \hat{e}_1 = -\theta_{11} \left( -\frac{1}{T_1} + \frac{1}{T_2} \right). \]


Structure of source terms (2)

Kinetic energy → Phenomenological coefficients

\[
\psi_{11} = \frac{1}{\tau_D} \frac{\rho_1 \rho_2}{\rho} T, \quad \theta_{11} = \frac{1}{\tau_T} \frac{\rho_1 c V_1 \rho_2 c V_2}{\rho_1 c V_1 + \rho_2 c V_2} T^2,
\]

\[
\frac{\tau_T}{\tau_D} = \frac{m_1 + m_2}{c m_2 + (1 - c) m_1}.
\]

\(\tau_D\) - relaxation time for diffusion
\(\tau_T\) - relaxation time for temperature
Parameters of the model (1)

Relaxation times

\[ \tau_D = \frac{cm_2 + (1 - c)m_1}{k_B T} D_{12}, \quad \tau_T = \frac{m_1 + m_2}{k_B T} D_{12}. \]

Diffusivity:

\[ D_{12} = \frac{3}{8n d_{12}^2} \left( \frac{k_B T}{2\pi} \frac{m_1 + m_2}{m_1 m_2} \right)^{1/2}, \quad n = n_1 + n_2 = \frac{\rho_1}{m_1} + \frac{\rho_2}{m_2} \]

- average atomic diameter of the mixture: \( d_{12} = \frac{d_1 + d_2}{2} \)
Parameters of the model (2)

Average mean free path:

\[ \lambda_0 = \frac{n_1}{n} (\lambda_1)_0 + \frac{n_2}{n} (\lambda_2)_0, \]

\[ (\lambda_\alpha)_0 = \frac{1}{\pi d_{12}^2} \left[ n_1 (1 + \frac{m_\alpha}{m_1})^{1/2} + n_2 (1 + \frac{m_\alpha}{m_2})^{1/2} \right]^{-1}. \]

Dimensionless quantities:

\[ \tilde{\rho} = \frac{\rho}{\rho_0}, \quad \tilde{u} = \frac{u}{a_0}, \quad \tilde{T} = \frac{T}{T_0}, \quad \tilde{J} = \frac{J}{\rho_0 a_0}, \quad \tilde{\Theta} = \frac{\Theta}{T_0}, \quad \tilde{\xi} = \frac{\xi}{\lambda_0}, \quad M_0 = \frac{u_0}{a_0}. \]

\[ \Pi_D = \frac{\lambda_0}{\tau_D a_0}, \quad \Pi_T = \frac{\lambda_0}{\tau_T a_0}. \]
Shock structure equations (1)

Traveling wave assumption → We seek for the solution in the form:

$$\psi(x, t) = \psi(x - st) = \psi(\xi)$$

- System of ODEs (Steady shock structure):

$$\frac{d}{d\xi} \mathbf{F}(\mathbf{U}, M_0, c_0, \mu) = \mathbf{P}(\mathbf{U}, M_0, c_0, \mu)$$

where

$$\mathbf{U} = (\rho, u, T, c, J, \Theta)^T$$

where $u = v_x - s$ relative velocity of the mixture with respect to wave front.
Shock wave structure in binary mixture for
\( t_\alpha = -p_\alpha l, \ q_\alpha = 0 \)

- **First look on shock structure**
- **Numerical simulation and experimental results**
- **Systematic analysis**
  - Shock thickness and Knudsen number
  - Temperature overshoot (TO)
Shock structure equations:

\[
\frac{d}{d\xi} (\rho u) = 0,
\]

\[
\frac{d}{d\xi} \left( \rho u^2 + \frac{1}{\gamma} \frac{m_0}{m} \rho T + \frac{J^2}{\rho c (1 - c)} \right) = 0,
\]

\[
\frac{d}{d\xi} \left\{ \left( \frac{1}{2} \rho u^2 + \frac{1}{\gamma - 1} \frac{m_0}{m} \rho T + \frac{J^2}{2 \rho c (1 - c)} \right) u + \left( \frac{uJ}{\rho c (1 - c) + \frac{1}{\beta}} \right) J \right\} = 0,
\]

\[
\frac{d}{d\xi} (\rho cu + J) = 0,
\]

\[
\frac{d}{d\xi} \left\{ \rho cu^2 + \frac{J^2}{\rho c} + 2uJ + \frac{1}{\gamma} \frac{m_0}{m_1} \rho c (T - f_1(c)\Theta) \right\} = -\frac{\lambda_0}{\tau_D a_0} m_\mu(T, c, \Theta) J,
\]

\[
\frac{d}{d\xi} \left\{ \left( \frac{1}{2} \rho c \left( u + \frac{J}{\rho c} \right)^2 + \frac{1}{\gamma - 1} \frac{m_0}{m_1} \rho c (T - f_1(c)\Theta) \right) \left( u + \frac{J}{\rho c} \right) \right\}
\]

\[
= -\frac{\lambda_0}{\tau_D a_0} m_\mu(T, c, \Theta) Ju - \frac{\lambda_0}{\tau_T a_0} e_\mu(\rho, T, c, \Theta) \Theta.
\]
Stationary points

\[ \mathbf{U}_0 = \lim_{\xi \to -\infty} \mathbf{U}(\xi), \quad \mathbf{U}_1 = \lim_{\xi \to +\infty} \mathbf{U}(\xi), \quad \lim_{\xi \to \pm\infty} \mathbf{U}'(\xi) = 0. \]

\[
\mathbf{U}_0 = \begin{bmatrix}
1 & 1 & 0 \\
M_0 & M_0 & 0 \\
c_0 & c_0 & 0 \\
0 & 0 & 0
\end{bmatrix}, \quad \mathbf{U}_1 = \begin{bmatrix}
\frac{4M_0^2}{3+M_0^2} & \frac{3+M_0^2}{4M_0} \\
16 \left(14 - \frac{3}{M_0^2} + 5M_0^2\right) & c_0 & 0 \\
0 & 0 & 0
\end{bmatrix}.
\]

Remark on numerical procedure:

1. Inviscid case → initial value problem
2. Viscous case → boundary value problem → finite difference
Constrains induced by the model

**Figure:** Critical values of $M_0$ and $\mu$ as a function of equilibrium concentration in front of the shock $c_0$
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Comparison with experimental results

Systematic analysis and results
Comparison with experimental results (1)

Velocity profiles \( \mu = 0.1, c_0 = 0.234, M_0 = 1.63 \)

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Comparison with experimental results (2)

Temperature profiles $\mu = 0.1, c_0 = 0.234, M_0 = 1.63$

Temperature overshoot:

$$TO = \frac{(T_2)_{\text{max}} - T_I}{T_I - T_0}$$
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Shock thickness and Knudsen number

\[ \delta = \left| \frac{u_1 - u_0}{(du/d\xi)_{\text{max}}} \right|, \quad \tilde{\delta} = \frac{\delta}{\lambda_0} = \frac{1}{Kn}. \]

- $Kn \lesssim 0.01$ – hydrodynamic flow
- $0.01 \lesssim Kn \lesssim 0.1$ – slip flow regime (slip flow regime)
- $0.1 \lesssim Kn \lesssim 10$ – transition flow regime $\rightarrow$ ET BE
- $Kn \gtrsim 10$ – free molecular flow regime $\rightarrow$ DSMC

Our results $\rightarrow$ Mesoscopic nature of the model

- Slip and transition flow: $0.002 \leq Kn \leq 0.48$
- Shock thickness: $\delta \approx (2 - 5)\lambda_0$
Kn → disipation, mixture structure (1)

\( c_0 = 0.41 \)
\( M_0 = 1.1 - 1.5 \)

\( c_0 = 0.59 \)
\( M_0 = 1.2 \)

**Figure:** Knudsen number as a function of mass ratio \( \mu \)
**Kn → dissipation, mixture structure (2)**

(a) $M_0 = 1.1 - 1.8$

(b) $M_0 = 1.1 - 1.5$

**Figure:** Knudsen number as a function of equilibrium concentration $c_0$
Non-monotonic behavior of TO (1)

Figure: TO as a function of mass ratio $\mu$

(a) $M_0 = 1.1 - 2.1$

(b) $M_0 = 1.1 - 1.5$
TO → non-monotonic behavior (2)

Figure: TO as a function of the equilibrium concentration $c_0$

(a) $M_0 = 1.1 - 1.6$

(b) $M_0 = 1.1 - 1.3$
Viscous model

Mixed type model

\[ \frac{\partial \rho_\alpha}{\partial t} + \text{div}(\rho_\alpha \mathbf{v}_\alpha) = \tau_\alpha, \]
\[ \frac{\partial (\rho_\alpha \mathbf{v}_\alpha)}{\partial t} + \text{div}(\rho_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha - \mathbf{t}_\alpha) = \mathbf{m}_\alpha, \]
\[ \frac{\partial \left( \frac{1}{2} \rho_\alpha \mathbf{v}_\alpha^2 + \rho_\alpha \varepsilon_\alpha \right)}{\partial t} + \text{div} \left\{ \left( \frac{1}{2} \rho_\alpha \mathbf{v}_\alpha^2 + \rho_\alpha \varepsilon_\alpha \right) \mathbf{v}_\alpha - \mathbf{t}_\alpha \mathbf{v}_\alpha + \mathbf{q}_\alpha \right\} = e_\alpha, \]

\[ \mathbf{q}_\alpha = -\kappa_\alpha \nabla T_\alpha, \quad \mathbf{t}_\alpha = -p_\alpha \mathbf{l} + \mu_\alpha \left( \nabla \mathbf{v}_\alpha + (\nabla \mathbf{v}_\alpha)^T \right) \]

Additional dissipation \( \rightarrow \)

\[ \text{DR} = \frac{d_1}{d_2} = \frac{d_{\text{He}}}{d_{\text{Ar}}} = 0.4366 \]
Shock structure equations (1)

1. \( \frac{d}{d\xi} (\rho u) = 0, \)

2. \( \frac{d}{d\xi} \left( \rho u^2 + \frac{1}{\gamma} \frac{m_0}{m} \rho T - \frac{1}{\gamma} \sigma^* + \frac{J^2}{\rho c(1-c)} \right) = 0, \)

3. \( \frac{d}{d\xi} \left\{ \left( \frac{1}{2} \rho u^2 + \frac{1}{\gamma-1} \frac{m_0}{m} \rho T + \frac{J^2}{2\rho c(1-c)} \right) u 
- \frac{1}{\gamma} \sigma^* u + \frac{1}{\gamma} q^* + \left[ \frac{u J}{\rho c(1-c)} - \frac{1}{\gamma} \left( \frac{\sigma_1}{\rho c} - \frac{\sigma_2}{\rho(1-c)} \right) + \frac{1}{\beta} \right] \right\} = 0, \)

4. \( \frac{d}{d\xi} (\rho cu + J) = 0, \)

5. \( \frac{d}{d\xi} \left\{ \rho cu^2 + \frac{J^2}{\rho c} + 2uJ + \frac{1}{m_0} \frac{m_0}{m_1} \rho c \left( T - f_1(c) \Theta - \frac{1}{\gamma} \sigma_1 \right) \right\} 
= -\frac{\lambda_0}{\tau_D a_0} m_\mu (T, c, \Theta) J, \)
Shock structure equations (2)

6. \[
\frac{d}{d\xi} \left\{ \left( \frac{1}{2} \rho c \left( u + \frac{J}{\rho c} \right)^2 + \frac{1}{\gamma - 1} m_0 \rho c \left( T - f_1(c)\Theta \right) \right) \left( u + \frac{J}{\rho c} \right) \right. \\
- \frac{1}{\gamma} \sigma_1 \left( u + \frac{J}{\rho c} \right) + \frac{1}{\gamma} q_1 \right\} = -\frac{\lambda_0}{\tau_D a_0} m_\mu(T, c, \Theta)Ju - \frac{\lambda_0}{\tau_T a_0} e_\mu(\rho, T, c, \Theta)\Theta
\]

7. \[
\frac{d}{d\xi} \left( u - \frac{J}{\rho c} \right) = \frac{3 \rho_0 a_0 \lambda_0}{4} \frac{\sigma_1}{\gamma \mu_{10}} \sqrt{T - f_1(c)\Theta}
\]

8. \[
\frac{d}{d\xi} \left( u - \frac{J}{\rho(1 - c)} \right) = \frac{3 \rho_0 a_0 \lambda_0}{4} \frac{\sigma_2}{\gamma \mu_{20}} \sqrt{T + f_2(c)\Theta}
\]

9. \[
\frac{d}{d\xi} (T - f_1(c)\Theta) = -\frac{\rho_0 a_0^3 \lambda_0}{\gamma T_0 \kappa_{10}} \frac{q_1}{\sqrt{T - f_1(c)\Theta}}
\]

10. \[
\frac{d}{d\xi} (T + f_2(c)\Theta) = -\frac{\rho_0 a_0^3 \lambda_0}{\gamma T_0 \kappa_{20}} \frac{q_2}{\sqrt{T + f_2(c)\Theta}}
\]
Kn, TO $\rightarrow$ dissipation mechanism influence

**Figure**: dashed line - viscous model, solid line - inviscid model
Comparison with finite-difference analysis of the Boltzmann equation

Molecular number densities: $\mu = 0.25, c_0 = 0.2, M_0 = 1.5, DR = 1, \frac{\lambda_K}{\lambda_0} = 1.057$

$$\lambda_K = \frac{1}{\sqrt{2\pi d^2 n_0}}$$

Summary

Main results

• Existence of TO,
• Non-monotonic dependence of the TO on mass ratio,
• straightforward numerics with time non-consuming procedures.

Open questions

• detailed study of numerical instabilities,
• seeking results for realistic gases in the case of high Mach numbers.