Multi-velocity and multi-temperature model of the mixture of polyatomic gases issuing from kinetic theory

Milana Pavić-Čolić

Department of Mathematics and Informatics
Faculty of Sciences, University of Novi Sad
Try Dostjeva Obradovića 4, 21000 Novi Sad, Serbia

Abstract

In this paper, we consider Euler-like balance laws for mixture components that involve macroscopic velocities and temperatures for each different species. These laws are not conservative due to mutual interaction between species. In particular, source terms that describe the rate of change of momentum and energy of the constituents appear. These source terms are computed with the help of kinetic theory for mixtures of polyatomic gases. Moreover, if we restrict the attention to processes which occur in the neighborhood of the average velocity and temperature of the mixture, the phenomenological coefficients of extended thermodynamics can be determined from the computed source terms.

Keywords: mixtures, polyatomic gases, kinetic theory, source terms, phenomenological coefficients

1. Introduction

We consider a mixture of $I$ polyatomic rarefied gases, denoted with $A_i$, $i = 1, \ldots, I$. We study the behavior of its components, since it is known that the behavior of a mixture as a whole at the macroscopic level can be very different from the behavior of its components when they are observed separately.

Within the continuum theories, the most sensitive question is about velocity and temperature field variables. In that sense, we distinguish between i) single-temperature approach [1], that stays within the framework of classical thermodynamics and assumes one macroscopic temperature of mixture and one macroscopic velocity and therefore, the state of the mixture is determined by the mass densities $\rho_i$ of each constituent, the mixture velocity $\mathbf{u}$ and the common temperature $T$, and ii) multi-temperature approach in the context of rational extended thermodynamics that introduces temperature $T_i$ and velocity $\mathbf{u}_i$ for each component of the mixture [12, 14].

Multi-velocity and multi-temperature models issuing from extended thermodynamics [13, 12], obey three principles proposed by Truesdell in [15], namely (i) all properties of the mixture must be mathematical consequences of properties of the constituents, (ii) to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, provided that we properly take into account for the actions of the other constituents upon it, (iii) the motion of the mixture is governed by the same equations as is a single body.

In particular, the second principle implies that each component of the mixture obeys balance laws of mass, momentum and energy, that are not conservative, because of the mutual interaction of the constituents. Thus, when chemical reactions are excluded from consideration, the following laws hold

$$\partial_t \rho_i + \nabla \cdot (\rho_i \mathbf{u}_i) = 0,$$

$$\partial_t (\rho_i \mathbf{u}_i) + \nabla \cdot (\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{p}_i) = \mathbf{N}_i,$$

$$\partial_t \rho_i \left( \frac{\mathbf{u}_i^2}{2} + e_i \right) + \nabla \cdot \left\{ \left( \rho_i \left( \frac{\mathbf{u}_i^2}{2} + e_i \right) \right) \mathbf{u}_i + \mathbf{q}_i \right\} = E_i,$$

for $i = 1, \ldots, I$, with $\rho_i$ being the density, $\mathbf{u}_i$ the velocity, $e_i$ the internal energy, $\mathbf{p}_i$ the pressure tensor and $\mathbf{q}_i$ the heat flux vector of the species $A_i$. The source terms $\mathbf{N}_i$ and $E_i$ correspond to momentum, respectively energy exchange.

In this paper we consider Eulerian fluids when off-diagonal parts of the pressure tensor and the heat flux vector vanish,

$$\mathbf{p}_i = \rho_i \mathbf{I}, \quad \mathbf{q}_i = 0, \quad i = 1, \ldots, I,$$

where $\rho_i$ is the hydrodynamic pressure of the constituent $A_i$, and $\mathbf{I}$ is the identity matrix.

The source terms $\mathbf{N}_i$ and $E_i$ need to satisfy the following relations

$$\sum_{i=1}^{I} \mathbf{N}_i = 0, \quad \sum_{i=1}^{I} E_i = 0,$$
since the first Truesdell’s principle asserts that the whole is just a sum of its parts, which means that we need to recover conservation laws of mass, momentum and energy for the mixture as a whole by summing equations 1. This is precisely achieved by imposing the restriction 3 and by defining

- mass density of mixture \( \rho = \sum_{i=1}^{I} \rho_i \),
- mixture velocity \( \mathbf{u} = \frac{1}{\rho} \sum_{i=1}^{I} \rho_i \mathbf{u}_i \),
- diffusion velocity \( \mathbf{U}_i = \mathbf{u}_i - \mathbf{u} \), with \( \sum_{i=1}^{I} \rho_i \mathbf{U}_i = 0 \),
- pressure tensor \( \mathbf{p} = \sum_{i=1}^{I} \left( \mathbf{p}_i + \rho_i \mathbf{u}_i \otimes \mathbf{u}_i \right) \),
- internal energy \( e = \frac{1}{\rho} \sum_{i=1}^{I} \rho_i \left( e_i + \frac{1}{2} \mathbf{U}_i ^2 \right) \),
- flux of internal energy

\[
\mathbf{q} = \sum_{i=1}^{I} \left( \left( \rho_i e_i + \frac{\rho_i}{2} \mathbf{U}_i ^2 + \mathbf{p}_i \right) \mathbf{U}_i + \mathbf{q}_i \right).
\]

Thus, summation of 1 over \( i = 1, \ldots, I \), yields conservation laws for the mixture

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{p}) &= 0, \\
\partial_t \left( \frac{\mathbf{u}}{2} \mathbf{u} ^2 + \rho e \right) + \nabla \cdot \left\{ \left( \frac{\mathbf{u}}{2} \mathbf{u} ^2 + \rho e \right) \mathbf{u} + \mathbf{p} \mathbf{u} + \mathbf{q} \right\} &= 0,
\end{align*}
\]

that are identical to those of a single fluid, according to the third principle.

With the assumption 2, the system 1 is still not closed, since we need to determine the source terms \( \mathbf{N}_i \) and \( \mathbf{E}_i \).

One approach to the closure problem is issuing from extended thermodynamics 13, where the objectivity and entropy principle are exploited in order to obtain their structure. The model consists of balance laws 1 for species \( \mathcal{A}_i \), \( i = 1, \ldots, I - 1 \) and mixture conservation laws 11 that replaces balance law for species \( \mathcal{A}_i \), together with the assumption 2 of Eulerian fluids. The source terms obtained in 13 are

\[
\begin{align*}
\mathbf{N}_i &= - \sum_{j=1}^{I-1} \alpha_{ij}(\mathbf{w}) \left( \frac{\mathbf{u}_i}{T_j} - \frac{\mathbf{u}_j}{T_i} - \mathbf{u} \left( \frac{1}{T_j} - \frac{1}{T_i} \right) \right), \\
\mathbf{E}_i &= \mathbf{u} \cdot \mathbf{N}_i - \sum_{j=1}^{I-1} \beta_{ij}(\mathbf{w}) \left( - \frac{1}{T_j} + \frac{1}{T_i} \right),
\end{align*}
\]

for all \( i = 1, \ldots, I - 1 \), where \( T_i \) is temperature of species \( \mathcal{A}_i \) (connected with pressure via \( p_i = n_i k T_i \), \( n_i \) is the number density and \( k \) is the Boltzmann constant), \( \alpha = [\alpha_{ij}]_{1 \leq i, j \leq I - 1} \) and \( \beta = [\beta_{ij}]_{1 \leq i, j \leq I - 1} \) are positive definite \((I - 1) \times (I - 1)\) matrix functions of the objective quantities \( \mathbf{w} \) (i.e. quantities invariant with respect to the Euclidean transformations). Thus, the given model contains phenomenological coefficients \( \alpha \) and \( \beta \), and extended thermodynamics does not provide any mean for their explicit determination.

On the other side, the source terms \( \mathbf{N}_i \) and \( \mathbf{E}_i \) can be determined using the kinetic theory of gases, provided that the collisional cross-section is specified. In particular, in 34 these source terms are calculated for some specific choices of the cross-section, and polyatomic gases are modeled with discrete energy levels.

The goal of this paper is to calculate the production terms \( \mathbf{N}_i \) and \( \mathbf{E}_i \) starting from the continuous internal energy model in the kinetic theory of gases from 2. Furthermore, the determined source terms are compared to the ones in 5 in order to derive explicit formula for phenomenological coefficients \( \alpha \) and \( \beta \) evaluated at the local equilibrium state.

The relation between extended thermodynamics of polyatomic gases and kinetic theory was analyzed in 2, 11, 14. So far, the analysis of phenomenological coefficients was successfully solved only at the level of binary mixture 9.

The plan of the paper is as follows. We present kinetic model in the Section 2 that allow us to compute the source terms in the Section 3. These source terms are compared to the ones coming out from extended thermodynamics in 1 in a linearized setting. In particular, we obtain phenomenological coefficients of thermodynamic model.

2. Kinetic Model for mixtures of polyatomic gases with continuous internal energy

In the kinetic theory, the state of mixture component \( \mathcal{A}_i \) is described by a distribution function \( f_i \geq 0 \), \( i = 1, \ldots, I \). In this paper, we follow the model with continuous internal energy presented in 3. Thus, the distribution function in this case, \( f_i := f_i(t, \mathbf{x}, \mathbf{v}, I) \), depends on time \( t \geq 0 \), space position \( \mathbf{x} \in \mathbb{R}^3 \), velocity \( \mathbf{v} \in \mathbb{R}^3 \) and the so-called microscopic internal energy \( I \geq 0 \), that aims at capturing all phenomena related to the polyatomic gas features (for example, rotations or vibrations during collision process).

In the kinetic theory style, the distribution function \( f_i \) changes due to the binary collisions with other particles of species \( \mathcal{A}_j \), \( j \in \{1, \ldots, I \} \). As a measure of its change, multi-species collision operators are introduced. Therefore, the evolution of the distribution function is governed
by the Boltzmann equation

$$\partial_t f_i + v \cdot \nabla_x f_i = \frac{1}{m_i} \sum_{j=1}^{I} Q_{ij}(f_i, f_j)(v, I), \quad 1 \leq i \leq I, \quad (6)$$

where $Q_{ij}(f_i, f_j)$ is the collision operator that describes interaction of molecules of species $A_i$ with molecules of species $A_j$ described by distribution function $f_j$. It reads

$$Q_{ij}(f_i, f_j)(v, I) = \int_{\mathbb{R}^3 \times \mathbb{R}^+ \times [0,1]^2 \times S^2} \left[ f'_j f''_j - f_i f_j \right] \times B_{ij} \left( 1 - R \right) R \frac{1}{\phi(I)} \, d\omega d\rho dI \, dv, \quad (7)$$

with standard abbreviations $f_j := f_j(t, x, v_s, I_s)$, $f'_j := f_j(t, x, v', I')$, $f''_j := f_j(t, x, v'', I'')$, where $v', v', I', I''$ are given in terms of $v, v_s, I, I_s$ and parameters $\omega \in S^2, r, R \in [0,1]$ via collisional rules

$$v' = G + \frac{m_i}{m_i + m_j} \left[ \frac{2 \mathbf{R} \cdot \mathbf{E}}{\mu_{ij}} \right] T_{c} \mathbf{g},$$

$$v'' = G - \frac{m_i}{m_i + m_j} \left[ \frac{2 \mathbf{R} \cdot \mathbf{E}}{\mu_{ij}} \right] T_{c} \mathbf{g},\quad (8)$$

$$I' = r(1 - R)E, \quad I'' = (1 - r)(1 - R)E,$$

with the total energy (kinetic plus microscopic internal energy) of the pair of particles during a collision

$$E := \mu_{ij} \frac{1}{2} \left| \mathbf{g} \right|^2 + I + I_s = \mu_{ij} \left| \mathbf{g} \right|^2 + I' + I'_s,$$

and where $G$ is a vector of center of mass $G := \frac{m_i v + m_j v_s}{m_i + m_j}$, $\mathbf{g}$ the relative velocity $g := v - v_s$, and $\mathbf{E}$ denotes the unit vector i.e. $\mathbf{g} := \mathbf{g}/|\mathbf{g}|$, $\mu_{ij}$ is the reduced mass $\mu_{ij} := \frac{m_i m_j}{m_i + m_j}$, and the mapping $T_{c} = 1 - 2(\omega \cdot \mathbf{z}) \mathbf{z}$, $\forall \mathbf{z} \in \mathbb{R}^3$. The cross section $B_{ij} := B_{ij}(v, v_s, I, I_s, r, R, \omega)$ is supposed to satisfy the micro-reversibility assumptions:

$$B_{ij}(v, v_s, I, I_s, r, R, \omega) = B_{ji}(v, v_s, I, I_s, r, R, \omega), \quad (9)$$

The test function $\varphi_i(I)$ will be chosen in order to recover perfect gas law for polyatomic gases in equilibrium.

### 2.1. Weak form of collision operator

Taking the moment of the collision operator (7) weighted with $\varphi_i(I)$ against some test function $\psi_i(v, I)$ yields

$$\int_{\mathbb{R}^3 \times \mathbb{R}^+} Q_{ij}(f_i, f_j)(v, I) \psi_i(v, I) \varphi_i(I) \, dI \, dv$$

$$= \int_{\mathbb{R}^3 \times \mathbb{R}^+ \times [0,1]^2 \times S^2} f_i f_j (\psi_i(v', I') - \psi_i(v, I)) \times B_{ij} \left( 1 - R \right) R \frac{1}{\phi(I)} \, d\omega d\rho dI \, dv, \quad (10)$$

### 2.2. Macroscopic quantities and conservation laws for mixtures

In order to recover macroscopic balance laws for mixture components $\Pi$ from the kinetic theory point of view, we first define macroscopic quantities. Mass density, momentum density and total energy density of the species $A_i$ are defined as the following moments of the distribution function:

$$\rho_i = \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{m_i}{m_i + m_j} \left( \int_{[0,1]^2 \times S^2} \frac{1}{\phi(I)} \, d\omega d\rho dI \right) \, dv$$

$$\rho_i u_i = \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{m_i}{m_i + m_j} \left( \int_{[0,1]^2 \times S^2} \frac{1}{\phi(I)} \, d\omega d\rho dI \right) v \, dv$$

$$\frac{1}{2} \rho_i |u_i|^2 + \rho_i \varepsilon_i = \int_{\mathbb{R}^3 \times \mathbb{R}^+} \frac{m_i}{m_i + m_j} \left( \int_{[0,1]^2 \times S^2} \frac{1}{\phi(I)} \, d\omega d\rho dI \right) \left( \frac{1}{2} v^2 + I \right) \, dv$$

If we introduce the peculiar velocity that corresponds to the species $A_i$, then pressure tensor and heat flux corresponding to the species $A_i$ are defined as follows

$$\left[ \rho_i \right]_{kk} q_k = \int_{\mathbb{R}^3 \times \mathbb{R}^+} \left( \frac{m_i}{m_i + m_j} \left( \int_{[0,1]^2 \times S^2} \frac{1}{\phi(I)} \, d\omega d\rho dI \right) v \right) \varphi_i(I) \, dv$$

Now, the macroscopic balance laws $\Pi$ can be obtained from the Boltzmann equation (6) in the following way: we integrate it with respect to $v \in \mathbb{R}^3$ and $I \in \mathbb{R}^+$, previously multiplying it with the test function $\varphi_i(I)$ and with (i) $\rho_i$ to obtain $\Pi_1$, (ii) $m_i v$ to get $\Pi_2$, and (iii) $(\frac{m_i}{m_i + m_j} |v|^2 + I)$ to obtain $\Pi_3$. Then production terms $N_i$ and $E_i$ are obtained as corresponding moments of the collision operator,

$$\left( \frac{N_i}{E_i} \right) = \int_{\mathbb{R}^3 \times \mathbb{R}^+} \left( \frac{m_i}{m_i + m_j} \left( \int_{[0,1]^2 \times S^2} \frac{1}{\phi(I)} \, d\omega d\rho dI \right) v \right) \varphi_i(I) \, dv$$

To fulfill assumptions of Eulerian fluids $\Pi$ we need to specify distribution function $f_i$, that will be done in the next Section.

### 3. Closure obtained from Kinetic Theory

We can close the set of equations $\Pi$ obtained also by kinetic theory in the previous Section, by means of the following steps:

i) The Eulerian fluids $\Pi$ can be obtained from definitions (12) by taking Maxwellian distribution function

$$M_i = \frac{n_i}{\rho_0(T_i)} \left( \frac{m_i}{2 \pi k T_i} \right)^{3/2} e^{-\frac{m_i}{2kT_i} (\frac{1}{2} |v-u|^2 + I)}, \quad (14)$$

with macroscopic number density $n_i = \rho_i/m_i$, macroscopic velocity $u_i$, and temperature $T_i$ (connected to the pressure via $p_i = n_i k T_i$, $k$ being the Boltzmann constant). Namely, plugging (14) into definition (12), we get that the pressure tensor
diagonalizes, with the coefficient \( n_i k T_i \) as a diagonal term, and the heat flux vector vanishes, as in (2).

This distribution function (14) corresponds to the “mid-equilibrium”, when the approach to equilibrium is divided into two processes [2]: i) the Maxwellisation step of a species – the approach of each distribution function to a Maxwellian distribution with its own velocity and temperature (\( f_i \to M_i \)), and ii) the equilibration of the species, i.e. vanishing of differences in velocity and temperature among the species.

ii) We choose the weight function \( \varphi_i(I) = I^{\alpha_i} \), with \( \alpha_i > -1 \) for every \( i = 1, \ldots, I \), so that the perfect gas law for polyatomic gases can be recovered

\[
\rho_i \varepsilon_i = \left( \alpha_i + \frac{5}{2} \right) k n_i T_i.
\]

In this case, the normalization constant in (13) reads

\[
\zeta_0(T_i) = \int_{\mathbb{R}_+} I^{\alpha_i} e^{-\frac{I}{k T_i}} dI = (k T_i)^{\alpha_i + 1} \Gamma [\alpha_i + 1].
\]

iii) We choose the following cross section

\[
B_{ji}(v, v_s, I, r, R, \omega) = 4 K R^{\gamma_{ji}} |g|^\gamma_{ji} |\omega \cdot \hat{g}|,
\]

(15)

\( g = v - v_s \), usually called the variable hard potential model with the parameter \( \gamma_{ij} \) that satisfies \( \gamma_{ij} = \gamma_{ji} \) and \( \gamma_{ij} > -\frac{3}{2} \), and \( K \) is an appropriate dimensional constant. The interest of this model is that it depends on one unique parameter \( \gamma_{ij} \) for each couple of species, which can be fitted by experiments involving only macroscopic quantities.

It remains to compute the production terms \( N_i \) and \( E_i \) for the choices above. They will be expressed in terms of hypergeometric function given in the Appendix A

3.1. Production term \( N_i \) for the momentum exchange

Using the weak form (19), the production term \( N_i \) from (13), that corresponds to the balance law of momentum of the species \( A_i \) for the Euler fluids and the cross section (15) reads

\[
N_i = \sum_{j=1}^{I} \int_{\mathbb{R}^2 \times [0,1]^2 \times S^2} m_i (v' - v) M_j M_{ji} \times 4 K (1 - R) R^{\gamma_{ji} + 1} |v - v_s|^{\gamma_{ji}} \times |\omega \cdot \hat{g}| \frac{d\omega}{|v - \hat{v_s}|} d\omega dR dI dI d\omega d\omega.
\]

Next we change angular variable \( \omega \rightarrow \sigma = g - 2 (\omega \cdot g) \omega \) with Jacobian obtained in (16)

\[
\int_{S^2} F(\sigma) d\sigma = \int_{S^2} F(2 - (\omega \cdot z) \omega) 2 |\omega \cdot z| d\omega,
\]

for all unit vectors \( z \), and for any function \( F \) such that the integrals are well defined. Expressing

\[
v' - v = m_j \frac{v + v_s + \sqrt{2 R E}}{m_i + m_j},
\]

the last integral becomes

\[
N_i = \sum_{j=1}^{I} K_{ij}^{1} \int_{\mathbb{R}^2 \times [0,1]^2 \times S^2} (v - v_s + \sqrt{2 RE}) \times e^{-\frac{m_j}{2 k T_s} |v - u_j|^2 + \frac{m_i}{2 k T_i} (|v - v_s|^2 + I)} (1 - R) R^{-\frac{\gamma_{ji} + 1}{2}} |v - v_s|^{\gamma_{ji}} d\sigma dR dI dI d\omega d\omega d\omega.
\]

Integration with respect to \( \sigma \), and then with respect to all variables except velocities \( v \) and \( v_s \), leads to:

\[
N_i = \sum_{j=1}^{I} K_{ij}^{1} \int_{\mathbb{R}^2 \times [0,1]^2 \times S^2} \times e^{-\frac{m_j}{2 k T_s} |v - u_j|^2 + \frac{m_i}{2 k T_i} (|v - v_s|^2 + I)} |v - v_s|^{\gamma_{ji}} d\sigma dR dI dI d\omega d\omega d\omega.
\]

Now we pass to the center of mass reference frame

\[
(v, v_s) \mapsto \left( g := v - v_s, G := \frac{m_i v + m_j v_s}{m_i + m_j} \right),
\]

(18)

with unit Jacobian. Then, integration with respect to \( G \) yields integrals which only involve the relative velocity \( g \):

\[
N_i = -\sum_{j=1}^{I} K_{ij}^{3} \int_{\mathbb{R}^3} g |g|^\gamma_{ji} e^{-a_{ij} g - (u_i - u_j)}^2 dg,
\]

(19)

with

\[
K_{ij}^{3} = K_{ij}^{1} k^2 T_i T_j \frac{16 \pi}{(3 + \gamma_{ij}) (5 + \gamma_{ij})},
\]

and

\[
a_{ij} = \left( \frac{k T_i}{m_i} + \frac{k T_j}{m_j} \right)^{-1}.
\]

In order to treat the scalar product of \( g \) and \( u_i - u_j \), we pass to spherical coordinates for \( g \) by taking \( u_i - u_j \) as a
zenith direction and an angle between \( \mathbf{g} \) and \( \mathbf{u}_i - \mathbf{u}_j \) as an azimuthal angle \( \theta \). Then, by parity arguments we have

\[
\int_{\mathbb{R}^3} |g|^{\gamma_{ij}} e^{-a_{ij}|g-(\mathbf{u}_i-\mathbf{u}_j)|^2} \, dg
= \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|} e^{-a_{ij}|\mathbf{u}_i - \mathbf{u}_j|^2} 2\pi \int_0^{\gamma_{ij} + 3} e^{-a_{ij}|g|^2} \times \int_0^\pi \cos \theta \, e^{2a_{ij}|\mathbf{u}_i - \mathbf{u}_j||g| \cos \theta} \sin \theta \, d\theta \, d|g|.
\]

The integral with respect to the angular variable \( \theta \) can be explicitly computed using special functions, we can write by means of the integral representation (A.3). Therefore, after using the weak form (14), reads

\[
E_i = \sum_{j=1}^{I} \int_{\mathbb{R}^3} |g|^{\gamma_{ij}} e^{-a_{ij}|g-(\mathbf{u}_i-\mathbf{u}_j)|^2} \, dg
\]

\[
= \frac{\mathbf{u}_i - \mathbf{u}_j}{|\mathbf{u}_i - \mathbf{u}_j|} e^{-a_{ij}|\mathbf{u}_i - \mathbf{u}_j|^2} 2\pi \int_0^{\gamma_{ij} + 3} e^{-a_{ij}|g|^2} \times \int_0^\pi \cos \theta \, e^{2a_{ij}|\mathbf{u}_i - \mathbf{u}_j||g| \cos \theta} \sin \theta \, d\theta \, d|g|.
\]

The term in the first parenthesis can be expressed in terms of non-prime variables as follows:

\[
\left[ -\frac{m_{ij}}{2} |\mathbf{v}'|^2 + I' - \frac{m_{ij}}{2} |\mathbf{v}|^2 - I \right] = -\mu_{ij} \mathbf{g} \cdot \mathbf{G} + \sqrt{2\mu_{ij} R E} \mathbf{g} \cdot \mathbf{T}_\omega [\mathbf{g}] + |\mathbf{g}|^2 \mu_{ij} \frac{1}{2} (1 - R) \left( -\frac{m_{ij}}{m_i + m_j} + r \right) + I \left( \frac{m_{ij}}{m_i + m_j} R + r (1 - R) \right) + I_* \left( \frac{m_{ij}}{m_i + m_j} R + r (1 - R) \right),
\]

by means of the integral representation (A.3). Therefore, we can write \( \mathbf{N}_i \) in closed form as follows

\[
\mathbf{N}_i = -\sum_{j=1}^{I} \Omega_{ij} \mathbf{N}_{ij}
\]

where the constant \( \Omega_{ij} \) is

\[
\Omega_{ij} = K \frac{n_{ij} k^{-(\alpha_i + \alpha_j)}}{\Gamma[\alpha_i + 1] \Gamma[\alpha_j + 1]} \frac{8 \pi \mu_{ij}}{\Gamma[\gamma_{ij} + 3]} \left[ \frac{\gamma_{ij} + 3}{2} \right].
\]

and

\[
\mathbf{N}_{ij} = (\mathbf{u}_i - \mathbf{u}_j) T^{-\alpha_i} T^{-\alpha_j} \times \left( \frac{2 T_i}{m_i} + \frac{2 T_j}{m_j} \right) e^{-\left( \frac{2 \mu_{ij} + 2 k T_i}{m_i} \right) \frac{1}{2} |\mathbf{u}_i - \mathbf{u}_j|^2} \times 1 F_1 \left( \frac{\gamma_{ij} + 5}{2} , \frac{5}{2} , \left( \frac{2 T_i}{m_i} + \frac{2 T_j}{m_j} \right) |\mathbf{u}_i - \mathbf{u}_j|^2 \right),
\]

where \( 1 F_1 \) is a hypergeometric function in (A.1).
with $a_{ij}$ from (20), and

\[
d_{ij} = \mu_{ij} \left( \frac{m_i}{2kT_i} + \frac{m_j}{2kT_j} \right)^{-1} \left( \frac{1}{2kT_i} - \frac{1}{2kT_j} \right),
\]

\[
e_{ij} = -\left( \frac{m_i}{2kT_i} + \frac{m_j}{2kT_j} \right)^{-1} \left( \frac{m_i}{2kT_i} u_i + \frac{m_j}{2kT_j} u_j \right).
\]

Comparing with (19), we recognize that the coefficient of $\delta_{ij}$ in (20), and using spherical coordinates for $g$, and calculating the integral with respect to the angular variable $\theta$

\[
\int_0^\pi e^{A_{ij}|g|\cos \theta} \sin \theta \, d\theta = \frac{2}{A_{ij} |g|} \sinh(A_{ij} |g|).
\]

with $A_{ij} = 2a_{ij} |u_i - u_j|$, we obtain

\[
E_i = \sum_{j=1}^{I} \sum_{j \neq i} \Omega_{ij} e_{ij} \cdot N_{ij} + \sum_{j=1}^{I} K_{ij} \frac{4\pi}{A_{ij}} e^{-a_{ij}|u_i - u_j|^2} \left\{ \begin{array}{l}
\int_{R^3} |g|^{\gamma_{ij} + 1+ \delta} e^{-a_{ij}|g|^2} \sinh(A_{ij} |g|) \, d|g| \\
\times \left\{ \begin{array}{l}
\left( \frac{m_i - m_j}{m_i + m_j} \right) (\gamma_{ij} + \frac{1}{2}) |g|^2 \\
+ \frac{m_i - m_j}{2\mu_{ij} (m_i + m_j)} (\gamma_{ij} + \frac{3}{2}) (kT_i + kT_j) \\
+ \frac{1}{2\mu_{ij}} (kT_j - kT_i) \end{array} \right. \\
\times \int_{R^3} |g|^{\gamma_{ij} + 1+ \delta} e^{-a_{ij}|g|^2} \sinh(A_{ij} |g|) \, d|g| \\
= \sqrt{\frac{\pi A_{ij}^{3/2}}{4a_{ij}} \gamma_{ij} + \delta + \frac{3}{2}} \left( \frac{\gamma_{ij} + \delta + \frac{3}{2}}{2} \right) \\
\times 1 \hat{F}_1 \left( \frac{\gamma_{ij} + \delta + \frac{3}{2}}{2}; \frac{3}{2} \right),
\end{array} \right.
\]

where $\delta = 2$ or $\delta = 0$, and $1 \hat{F}_1$ is a hypergeometric function defined in (A.11). Substituting the coefficients, we get the final expression for the production term that corresponds to the energy balance law of the species $A_i$ of Euler fluids, for the cross section (15).

\[
E_i = - \sum_{j=1}^{I} \sum_{j \neq i} \Omega_{ij} \left( \frac{m_i}{2kT_i} + \frac{m_j}{2kT_j} \right)^{-1} \left( \frac{1}{2kT_i} - \frac{1}{2kT_j} \right) \cdot N_{ij} \\
+ \sum_{j=1}^{I} \frac{2\Omega_{ij}}{(\gamma_{ij} + 3)(r^a_{ij} - a_{ij})} \left( \frac{2kT_i}{m_i} + \frac{2kT_j}{m_j} \right)^{2\nu} \\
\times e^{-\frac{2\nu kT_i}{m_i} + \frac{2\nu kT_j}{m_j}} |u_i - u_j|^2 \left\{ \begin{array}{l}
\left( \frac{m_i}{2kT_i} + \frac{m_j}{2kT_j} \right) (\gamma_{ij} + \frac{3}{2}) \\
\times \left( \mu_{ij} \frac{T_i - T_j}{m_i T_j + m_j T_i} + \frac{m_i - m_j}{(m_i + m_j)} (\gamma_{ij} + \frac{7}{2}) \right) \\
\times \left( \frac{m_i - m_j}{2\mu_{ij} (m_i + m_j)} (\gamma_{ij} + \frac{3}{2}) (kT_i + kT_j) + \frac{m_i - m_j}{2\mu_{ij}} (kT_j - kT_i) \right) \\
\times \int_{R^3} |g|^{\gamma_{ij} + 1+ \delta} e^{-a_{ij}|g|^2} \sinh(A_{ij} |g|) \, d|g| \\
= \sqrt{\frac{\pi A_{ij}^{3/2}}{4a_{ij}} \gamma_{ij} + \delta + \frac{3}{2}} \left( \frac{\gamma_{ij} + \delta + \frac{3}{2}}{2} \right) \\
\times 1 \hat{F}_1 \left( \frac{\gamma_{ij} + \delta + \frac{3}{2}}{2}; \frac{3}{2} \right),
\end{array} \right.
\]

with constant $\Omega_{ij}$ from (23).

4. Comparison with the model issuing from Extended Thermodynamics in the linearized setting

The aim of this section is to compare source terms (22) and (25) that we have calculated using the kinetic theory of gases with the source terms (5) obtained thanks to extended thermodynamics.

Even though we restricted the attention to the description at the Euler level, this comparison is not possible in general, since the source terms have a completely different non-linear structure. However, they can be reduced to considerably simpler form, if we restrict the attention to processes which occur in the neighborhood of local equilibrium state determined by the average velocity $u_i = u$ and the average temperature $T = T$ of the mixture. Under this assumption, we can linearize the source terms

\[
A := A(u_i, u_j, T_i, T_j) \approx A(u, u, T, T) \\
+ \nabla A(u, u, T, T) \cdot [u_i - u, u_j - u, T_i - T, T_j - T]^T,
\]

for $A$ equal to $N_i$ or $E_i$, which holds when $(u_i, u_j, T_i, T_j)$ is close to $(u, u, T, T)$, for any $i, j = 1, \ldots, I$.

Source terms (5) issuing from extended thermodynamics
can be rewritten and then approximated by

\[ N_i \approx \sum_{j=1 \atop j \neq i}^I A_{ij}(w^0) (u_j - u_i), \]

\[ E_i \approx u \cdot \sum_{j=1 \atop j \neq i}^I A_{ij}(w^0) (u_j - u_i) + \sum_{j=1 \atop j \neq i}^I B_{ij}(w^0) (T_j - T_i), \]

where \( w^0 := w(u, u, T, T) \) denotes an objective quantity \( w(u, u, T, T) \) evaluated at \((u, u, T, T)\), and the coefficients are

\[
A_{ij}(w^0) = \begin{cases} \frac{-1}{2} \alpha_{ij}(w^0), & j = 1, \ldots, I - 1, j \neq i, \\ \sum_{k=1}^{I-1} \alpha_{ik}(w^0), & j = I, \end{cases}
\]

\[
B_{ij}(w^0) = \begin{cases} \frac{-1}{2} \beta_{ij}(w^0), & j = 1, \ldots, I - 1, j \neq i, \\ \sum_{k=1}^{I-1} \beta_{ik}(w^0), & j = I. \end{cases}
\]

Approximating source terms (22) and (25) coming from kinetic theory, we obtain

\[ N_i \approx \sum_{j=1 \atop j \neq i}^I C_{ij} \frac{2 \mu_{ij}}{3} (u_j - u_i), \]

\[ E_i \approx u \cdot \sum_{j=1 \atop j \neq i}^I C_{ij} \frac{2 \mu_{ij}}{3} (u_j - u_i) \]

\[
+ \sum_{j=1 \atop j \neq i}^I C_{ij} \frac{2 (\gamma_{ij} + 5)}{(\gamma_{ij} + 7)} \left( \frac{1}{(\gamma_{ij} + 3)} + \frac{\mu_{ij}}{(m_i + m_j)} \right) k(T_j - T_i), \]

\[ (27) \]

where

\[ C_{ij} = \frac{\mu_{ij}}{2} \frac{16K \sqrt{\pi}}{(\gamma_{ij} + 5) \Gamma[\alpha_i + 1] \Gamma[1 + \alpha_j + 1]} \left( kT \right)^{-(\alpha_i + \alpha_j + \frac{1}{2})} \]

Then (24) and (25) can be directly compared to obtain explicit expressions for matrices \( \alpha \) and \( \beta \) in local equilibrium. First, we obtain the off-diagonal terms:

\[
\alpha_{ij}(w^0) = -C_{ij} \frac{2 \mu_{ij}}{3} kT, \]

\[
\beta_{ij}(w^0) = -C_{ij} \frac{2 (\gamma_{ij} + 5)}{(\gamma_{ij} + 7)} \left( \frac{1}{(\gamma_{ij} + 3)} + \frac{\mu_{ij}}{(m_i + m_j)} \right) kT^2 \]

for any \( i = 1, \ldots, I - 1 \) and for \( 1 \leq j \leq I - 1 \) such that \( j \neq i \). Next, we get the diagonal terms:

\[
\alpha_{ii}(w^0) = -\sum_{\ell=1 \atop \ell \neq i}^I \alpha_{i\ell}(w^0) = \sum_{\ell=1 \atop \ell \neq i}^I C_{i\ell} \frac{2 \mu_{i\ell}}{3} kT, \]

\[
\beta_{ii}(w^0) = -\sum_{\ell=1 \atop \ell \neq i}^I \beta_{i\ell}(w^0) = \sum_{\ell=1 \atop \ell \neq i}^I C_{i\ell} \frac{2 (\gamma_{i\ell} + 5)}{(\gamma_{i\ell} + 7)} \left( \frac{1}{(\gamma_{i\ell} + 3)} + \frac{\mu_{i\ell}}{(m_i + m_{\ell})} \right) kT^2 \]

where \( i = 1, \ldots, I - 1 \).

We need to check positive definiteness of obtained matrices \( \alpha \) and \( \beta \). Since their structure is the same, we will provide the proof for \( \alpha \). Notice that the matrix \( \alpha \) is symmetric and to show its positive definiteness we use Sylvester’s criterion. Firstly, the principal minor of order one is clearly positive,

\[ M_1 = \alpha_{11} > 0. \]

Then, the leading principal minor of order \( k, M_k \), with \( k = 2, \ldots, I - 1 \) (for \( k = I - 1 \) we obtain \( \alpha \) itself), can be represented as a determinant of a sum of two matrices by separating terms on diagonal. Namely,

\[ M_k = \det (\alpha_k^0 + \alpha_k^d). \]

where the elements of \( \alpha_k^0 \) are given with

\[ \alpha_{k,i,j}^0 = \begin{cases} \alpha_{ij}, & \text{if } i \neq j, \\ -\sum_{k=1 \atop k \neq i}^{I-1} \alpha_{ik}, & \text{if } i = j, \end{cases} \]

for \( i, j = 1, \ldots, k \), and the diagonal matrix \( \alpha^d \) is given by its elements

\[ \alpha_{k,i,j}^d = -\sum_{\ell=1}^{k+1} \alpha_{i\ell} \delta_{ij}, \]

\( \delta_{ij} \) being the Kronecker delta.

Considering the determinant of matrix \( \alpha_k^0 \), we add all columns to the first one, or equivalently we add all rows to the first one, and obtain zeros on the first column (row), and therefore \( \alpha_k^0 \) has zero determinant for any \( k \). On the other side, \( \alpha_k^d \) is a diagonal matrix with all positive terms, and thus its determinant is positive for any \( k \). Therefore, since the determinant of two positive semi-definite matrices is greater or equal than the sum of the two corresponding determinants [10] (p. 228), we conclude that for any \( k = 2, \ldots, I - 1 \) it holds

\[ M_k \geq \det \alpha_k^0 + \det \alpha_k^d > 0, \]

which implies that \( \alpha \) is positive definite matrix.
Therefore, we have determined the phenomenological coefficients $\alpha$ and $\beta$ of extended thermodynamics \cite{Arima} for $u_i = u$ and $T_i = T$, $i = 1, \ldots, I$, from the source terms provided by the kinetic theory. These are important results in further application of the multi-temperature model. For instance, when considering the shock profile solutions, as in \cite{Bisi2,Bisi3}.

5. Acknowledgment

The author would like to thank Professor Laurent Desvillettes and Professor Srboljub Simić for many fruitful discussions and inputs for this work. This research is supported by the Project No. ON174016 of Ministry of Education, Science and Technological Development, Republic of Serbia.

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\end{enumerate}

Appendix A. Hypergeometric functions

We introduce the regularized Kummer confluent hypergeometric function, denoted by $\tilde{1}\tilde{F}_1(a,b,z)$, with its integral representation

$$\Gamma [b - a] \Gamma [a] \tilde{1}\tilde{F}_1(a,b,z) = \int_0^1 e^{zt} t^{a-1} (1-t)^{b-a-1} dt, \quad (A.1)$$

for $b > a > 0$, see \cite{Abramowitz} p. 505, relation 13.2.1. Next, we introduce the following function

$$0\tilde{F}_1(b,z) = \frac{1}{\Gamma [b]} e^{-2\sqrt{z}} \tilde{1}\tilde{F}_1(b - \frac{1}{2},2b - 1,4\sqrt{z}). \quad (A.2)$$

The two hypergeometric functions are connected through the integral representation

$$\tilde{1}\tilde{F}_1(a,b,z) = \frac{1}{\Gamma [a]} \int_0^\infty e^{-t} t^{a-1} 0\tilde{F}_1(b,zt) dt, \quad (A.3)$$

for $a > 0$. 
