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Six-Field Theory for a Polyatomic Gas Mixture: Extended Thermodynamics and Kinetic Models

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Abstract: Polyatomic gases may be characterized by internal molecular degrees of freedom. As a consequence, at a macroscopic level, dynamic pressure appears, which may be related to the bulk viscosity of the gas. Inspired by the models of a single polyatomic gas with six fields, developed within rational extended thermodynamics (RET) and the kinetic theory of gases, this paper presents a six-field theory for the mixture of polyatomic gases. First, the macroscopic mixture model is developed within the framework of RET. Second, the mixture of gases with six fields is analyzed in the context of the kinetic theory of gases, and corresponding moment equations are derived. Finally, complete closure of the RET model, i.e., computation of the phenomenological coefficients, is achieved by means of a combined macroscopic/kinetic closure procedure.

Keywords: mixture; polyatomic gases; dynamic pressure; six-field model; extended thermodynamics; kinetic theory

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1. Introduction

Mixtures are media that consist of several identifiable constituents. Vast amounts of materials occurring in nature, engineering, and technological processes may be regarded as mixtures. Therefore, mixture modeling is an important and demanding task.

The modeling of gaseous mixtures may follow different paths. The macroscopic or continuum approach is based upon the balance laws of continuum mechanics and may be different depending on the choice of field variables used to describe the state of the mixture. A coherent macroscopic description of mixtures compatible with fundamental physical principles is presented in [1]. It is a classical model which relies on generalized Fick's law of diffusion. A comprehensive account of multicomponent mixtures may be found in [2,3]. However, within the framework of rational extended thermodynamics (RET), [4] a model is developed which goes beyond the classical approach and aims to remove the paradox of infinite speed of wave propagation. On one hand, it resonates with the principles of rational thermodynamics [5], while on the other hand, extends the list of field variables by introducing the velocities of constituents. This model was further extended to a so-called multi-temperature mixture [6,7]. It was then analyzed for its comparison with the classical approach [8–10] and applied to non-equilibrium processes in mixtures [11–13].

Mixtures of gases can be studied equally well starting from the kinetic theory of gases. In this (mesoscopic) approach, one firstly relies on the system of Boltzmann equations for mixture and the choice of the model of interaction between the particles. In the next step, corresponding macroscopic equations for the chosen set of field variables are derived as moment equations using the standard moment method [14]. This procedure requires the approximation of a distribution function that is compatible with the choice of field variables, which can be done in several ways—classical Grad's method [15] and the maximum entropy principle [16–18] are examples of this procedure. It is remarkable that under certain assumptions about the interaction of the species one may derive the moment equations of the multi-temperature model, which are compatible with the model of extended thermodynamics [19].

Although macroscopic and kinetic approaches to gaseous mixtures seem to converge in a certain way, there are some open problems that are the subject of analysis in either context. First, the modeling of polyatomic gases became a topic of intensive research in RET and kinetic theory in the last decade. Major achievements of extended thermodynamics in this problem were summarized in [20,21], whereas certain results about kinetic modeling of polyatomic gases may be found in [22,23]. On the other hand, the description of dissipation in polyatomic gases is a delicate problem, both in RET and in kinetic theory, and strongly depends on the level of approximation. Apart from the 14-moment description of polyatomic gases [24–28] and recently 17-moment [29,30], there appeared a simplified 6-moment model, the simplest model which captures the non-equilibrium effects through a single field variable—dynamic pressure [31]. This model is particularly interesting because it allows an exact closure, both in macroscopic and kinetic framework [27,32–34]. Moreover, it is relevant in applications for describing non-equilibrium gas flows with large bulk viscosity. For instance, it is observed that CO_2 has a relaxation time for dynamical pressure much larger than relaxation times for stress tensor and heat flux [35–37]. The aim of this study is to use this model as a starting point and build up a model of gaseous mixtures in which each constituent is described by the six fields.

In this paper, we shall develop a six-field theory for polyatomic gases, both in macroscopic and kinetic contexts. In the macroscopic description, we shall rely on the methods of RET, postulate the structure of field equations, use the objectivity principle to give an insight into the basic ingredients of equations, and apply the entropy principle to choose the admissible set of constitutive relations. In the kinetic description, we shall apply the maximum entropy principle to derive the approximate form of distribution function compatible with macroscopic field variables, and derive the field equations as moment equations for the system of Boltzmann equations for a polyatomic gas mixture. In particular, for the computation of source terms, the collision kernel satisfying assumptions from the rigorous mathematical analysis established in [38,39] is used. These two approaches do not match completely since the source terms do not have the same form. Moreover, RET source terms are not entirely determined since they comprise phenomenological coefficients whose form is not prescribed. To that end, we shall apply the recently introduced macroscopic/kinetic closure procedure [40,41] to determine the phenomenological coefficients of RET by matching the macroscopic and the kinetic source terms in the neighborhood of local equilibrium manifold, i.e., in their linearized version.

The rest of the paper is organized as follows. In Section 2, we present the macroscopic approach to mixture modeling within the framework of RET. In Section 3, the kinetic model of mixtures is presented and corresponding moment equations are derived. Section 4 contains a combined macroscopic/kinetic closure of governing equations and provides the structure of phenomenological coefficients of RET. The paper is concluded with a review of results and further outlook.

2. Macroscopic Model of the Mixture with Dynamic Pressure

In this section, we shall first give a brief recap of the single-component polyatomic gas model with dynamic pressure, usually denoted as the ET6 model [20,21]. After that, an analysis of macroscopic equations for the mixture of polyatomic gases will be provided. Finally, an analysis of constitutive relations through the application of objectivity and entropy principles will be given.

2.1. Macroscopic Model of a Single-Component Polyatomic Gas

Let us first emphasize that Latin indices denote Cartesian components of vectors and tensors and the summation convention is assumed, that is, when exactly two Latin indices are repeated in the expression, it means that we take the sum over that index. The governing equations of the ET6 model for polyatomic gases read:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k}(\rho v_k) = 0, \\
&\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_k}(\rho v_i v_k - t_{ik}) = 0, \quad (i = 1, 2, 3) \\
&\frac{\partial}{\partial t}\left(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho\varepsilon\right), \\
&\quad + \frac{\partial}{\partial x_k}\left\{\left(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho\varepsilon\right)v_k - t_{ki}v_i + q_k\right\} = 0, \\
&\frac{\partial}{\partial t}\left\{\rho|\mathbf{v}|^2 + 3(p + \Pi)\right\} + \frac{\partial}{\partial x_k}F_{llk} = P,
\end{aligned} \tag{1}$$

where ρ is the mass density, v_k is the velocity, ε is the specific internal energy, t_{ik} is the stress tensor, q_k is the heat flux, and the flux F_{llk} is determined by:

$$F_{llk} = \left[\rho|\mathbf{v}|^2 + 5(p + \Pi)\right]v_k, \tag{2}$$

while the following constitutive assumptions are taken for the non-convective fluxes:

$$t_{ik} = -(p + \Pi)\delta_{ik}, \quad q_k = 0, \tag{3}$$

where $p(\rho, \varepsilon)$ is the hydrostatic pressure, and Π is the dynamic pressure. In $(1)_4$ P is the source term of relaxation type.

The entropy density of the gas described with six fields has the form:

$$h = \rho s + \rho k, \tag{4}$$

where $s = s(\rho, \varepsilon)$ is the equilibrium-specific entropy, while $k = k(\rho, \varepsilon, \Pi)$ is the non-equilibrium specific entropy, which satisfies the equilibrium condition $k(\rho, \varepsilon, 0) = 0$. Application of the entropy principle yields the residual inequality

$$\Sigma = \frac{1}{3}\rho\frac{\partial k}{\partial \Pi}P > 0, \tag{5}$$

which is satisfied, for example, when the source term is expressed in terms of non-equilibrium specific entropy as follows

$$P = \alpha\frac{\partial k}{\partial \Pi}, \tag{6}$$

where $\alpha \geq 0$ is the function of objective quantities. Additionally, k must satisfy the following PDE:

$$\rho^2\frac{\partial k}{\partial \rho} + (p + \Pi)\frac{\partial k}{\partial \varepsilon} + \rho\left\{-\rho\frac{\partial p}{\partial \rho} + (p + \Pi)\left(\frac{5}{3} - \frac{1}{\rho}\frac{\partial p}{\partial \varepsilon}\right)\right\}\frac{\partial k}{\partial \Pi} + \frac{\Pi}{T} = 0. \tag{7}$$

It was shown that there exists a general solution of this equation that satisfies the equilibrium condition, and that in the case of polytropic gases it is expressed in terms of a single variable, Π/p,

$$k = \frac{k_{\mathrm{B}}}{m}\log\left\{X^{3/2}\,Y^{a+1}\right\}; \quad X = 1 + \frac{\Pi}{p}, \quad Y = 1 - \frac{3}{2(a+1)}\frac{\Pi}{p}, \tag{8}$$

where k_{B} is the Boltzmann constant and m the molecular mass. Parameter $a > -1$ can be related to the number of molecular degrees of freedom D, $a = (D - 5)/2$.

These results were confirmed for a single-component polyatomic gas starting from the kinetic theory and the Boltzmann equation. Namely, on one side, the non-equilibrium specific entropy k is constructed as a moment of the distribution function and is shown that PDE (7) is satisfied [33]. Moreover, the dynamic pressure source term P is explicitly calculated and the residual inequality (5) is recovered [27].

2.2. Governing Equations for the Mixture of Polyatomic Gases

A macroscopic approach to mixture modeling is based on Truesdell's metaphysical principles. In the framework of RET, their application has to be adapted to the mixture of polyatomic gases, in which only the dynamic pressures are taken as non-equilibrium variables. Therefore, the behavior of the constituents is governed by the same equations as for the single fluid, taking into account the mutual interaction with other constituents through the source terms:

$$\begin{aligned}
&\frac{\partial \rho_\alpha}{\partial t} + \frac{\partial}{\partial x_k}(\rho_\alpha v_{\alpha k}) = \tau_\alpha, \\
&\frac{\partial}{\partial t}(\rho_\alpha v_{\alpha i}) + \frac{\partial}{\partial x_k}(\rho_\alpha v_{\alpha i} v_{\alpha k} - t_{\alpha ik}) = m_{\alpha i}, \quad (i = 1,2,3) \\
&\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_\alpha |\mathbf{v}_\alpha|^2 + \rho_\alpha \varepsilon_\alpha\right), \\
&\quad + \frac{\partial}{\partial x_k}\left\{\left(\frac{1}{2}\rho_\alpha |\mathbf{v}_\alpha|^2 + \rho_\alpha \varepsilon_\alpha\right) v_{\alpha k} - t_{\alpha ki} v_{\alpha i} + q_{\alpha k}\right\} = e_\alpha, \\
&\frac{\partial}{\partial t}\left\{\rho_\alpha |\mathbf{v}_\alpha|^2 + 3(p_\alpha + \Pi_\alpha)\right\} \\
&\quad + \frac{\partial}{\partial x_k}\left\{\left[\rho_\alpha |\mathbf{v}_\alpha|^2 + 5(p_\alpha + \Pi_\alpha)\right] v_{\alpha k}\right\} = P_\alpha + M_\alpha.
\end{aligned} \tag{9}$$

In Equation (9), Greek index $\alpha = 1, \dots, n$ stands for the constituent; τ_α, $m_{\alpha i}$, e_α, and M_α are the interaction source terms, whereas P_α is the internal dissipative source term for dynamic pressure of the constituent α. Let us highlight that the summation convention does not apply to Greek letters. For instance,

$$t_{\alpha ki} v_{\alpha i} \qquad \text{stands for} \qquad \sum_{i=1}^{3} t_{\alpha ki} v_{\alpha i}, \tag{10}$$

i.e., the summation is assumed only over exactly two repeated Latin indices i and not over α.

In this model, field variables that describe the state of the mixture are:

$$\tilde{\mathbf{u}} = (\rho_\alpha, \mathbf{v}_\alpha, \varepsilon_\alpha, \Pi_\alpha). \tag{11}$$

Following the principles of RET, all the constitutive functions have to be locally expressed in terms of variables $\tilde{\mathbf{u}}$, i.e., they should depend on their local values in point, but not on the values of their derivatives.

Truesdell's principles also state that governing equations for the whole mixture have the same form as equations for the single fluid, where macroscopic densities and fluxes for the mixture have to be properly defined in terms of densities and fluxes of the constituents. To that end, the interaction source terms must satisfy the conservation axioms:

$$\sum_{\alpha=1}^{n} \tau_\alpha = 0; \quad \sum_{\alpha=1}^{n} m_{\alpha i} = 0; \quad \sum_{\alpha=1}^{n} e_\alpha = 0; \quad \sum_{\alpha=1}^{n} M_\alpha = 0. \tag{12}$$

However, the sum of internal dissipative source terms P_α does not disappear but represents the dissipative source term for the dynamic pressure of the mixture:

$$\sum_{\alpha=1}^{n} P_\alpha =: P. \tag{13}$$

Summation of the corresponding balance laws (9) for the constituents lead to the governing equations for the mixture in the form (1), where the mixture densities and fluxes are defined as:

$$\begin{aligned}
&\rho = \sum_{\alpha=1}^{n} \rho_\alpha; \quad \rho v_i = \sum_{\alpha=1}^{n} \rho_\alpha v_{\alpha i}; \quad u_{\alpha i} = v_{\alpha i} - v_i; \\
&\rho\varepsilon = \sum_{\alpha=1}^{n} \left\{ \rho_\alpha \varepsilon_\alpha + \frac{1}{2}\rho_\alpha |\mathbf{u}_\alpha|^2 \right\}; \\
&p = \sum_{\alpha=1}^{n} p_\alpha; \quad \Pi = \sum_{\alpha=1}^{n} \left(\Pi_\alpha + \frac{1}{3}\rho_\alpha |\mathbf{u}_\alpha|^2 \right); \\
&t_{ij} = \sum_{\alpha=1}^{n} \{ t_{\alpha ij} - \rho_\alpha u_{\alpha i} u_{\alpha j} \}; \\
&q_i = \sum_{\alpha=1}^{n} \left\{ q_{\alpha i} - t_{\alpha ij} u_{\alpha j} + \left(\frac{1}{2}\rho_\alpha |\mathbf{u}_\alpha|^2 + \rho_\alpha \varepsilon_\alpha \right) u_{\alpha i} \right\}; \\
&F_{llk} = \rho |\mathbf{v}|^2 v_k + 5(p+\Pi) v_k + 2 v_l \hat{U}_{\langle lk \rangle} + \hat{F}_{llk},
\end{aligned} \tag{14}$$

where:

$$\begin{aligned}
\hat{U}_{\langle lk \rangle} &= \sum_{\alpha=1}^{n} \left\{ \rho_\alpha \left(u_{\alpha l} u_{\alpha k} - \frac{1}{3} |\mathbf{u}_\alpha|^2 \delta_{lk} \right) \right\}; \\
\hat{F}_{llk} &= \sum_{\alpha=1}^{n} \left\{ \rho_\alpha |\mathbf{u}_\alpha|^2 u_{\alpha k} + 5(p_\alpha + \Pi_\alpha) u_{\alpha k} \right\}.
\end{aligned} \tag{15}$$

In (14), $u_{\alpha i}$ is the diffusion velocity, and the following identity holds, $\sum_{\alpha=1}^{n} \rho_\alpha u_{\alpha i} = 0$. Since our analysis is restricted to the polyatomic gases with dynamic pressure, we introduce the following constitutive assumptions for partial stress tensors and partial heat fluxes:

$$t_{\alpha ij} = -(p_\alpha + \Pi_\alpha)\delta_{ij}; \quad q_{\alpha i} = 0, \tag{16}$$

where $p_\alpha(\rho_\alpha, \varepsilon_\alpha)$ are the partial thermodynamic pressures, and Π_α are the partial dynamic pressures. As a consequence, the stress tensor t_{ij} and the internal energy flux q_i of the mixture reduce to:

$$\begin{aligned}
t_{ij} &= -\sum_{\alpha=1}^{n} \{ (p_\alpha + \Pi_\alpha)\delta_{ij} + \rho_\alpha u_{\alpha i} u_{\alpha j} \}; \\
q_i &= \sum_{\alpha=1}^{n} \left\{ (p_\alpha + \Pi_\alpha) u_{\alpha i} + \left(\frac{1}{2}\rho_\alpha |\mathbf{u}_\alpha|^2 + \rho_\alpha \varepsilon_\alpha \right) u_{\alpha i} \right\}.
\end{aligned} \tag{17}$$

In the mixture theory, it is usual to construct the system of governing equations by replacing the balance laws for one constituent, say $\alpha = n$, with the governing equations for the whole mixture. Therefore, we list the system of governing equations that will be used in the sequel, which consists of a mixture governing of equations:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k}(\rho v_k) = 0, \\
&\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_k}(\rho v_i v_k - t_{ik}) = 0, \quad (i = 1,2,3) \\
&\frac{\partial}{\partial t}\left(\frac{1}{2}\rho |\mathbf{v}|^2 + \rho\varepsilon \right) + \frac{\partial}{\partial x_k}\left\{ \left(\frac{1}{2}\rho |\mathbf{v}|^2 + \rho\varepsilon \right) v_k - t_{ki} v_i + q_k \right\} = 0, \\
&\frac{\partial}{\partial t}\left\{ \rho |\mathbf{v}|^2 + 3(p+\Pi) \right\} + \frac{\partial}{\partial x_k} F_{llk} = P,
\end{aligned} \tag{18}$$

and the balance laws for $n-1$ constituents:

$$
\begin{aligned}
&\frac{\partial \rho_b}{\partial t} + \frac{\partial}{\partial x_k}(\rho_b(v_k + u_{bk})) = \tau_b, \\
&\frac{\partial}{\partial t}(\rho_b(v_i + u_{bi})) + \frac{\partial}{\partial x_k}(\rho_b(v_i + u_{bi})(v_k + u_{bk}) - t_{bik}) = m_{bi}, \quad (i = 1,2,3) \\
&\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_b|\mathbf{v} + \mathbf{u}_b|^2 + \rho_b \varepsilon_b\right), \\
&\quad + \frac{\partial}{\partial x_k}\left\{\left(\frac{1}{2}\rho_b|\mathbf{v} + \mathbf{u}_b|^2 + \rho_b \varepsilon_b\right)(v_k + u_{bk}) - t_{bki}(v_k + u_{bk}) + q_{bk}\right\} = e_b, \\
&\frac{\partial}{\partial t}\left\{\rho_b|\mathbf{v} + \mathbf{u}_b|^2 + 3(p_b + \Pi_b)\right\} \\
&\quad + \frac{\partial}{\partial x_k}\left\{\left[\rho_b|\mathbf{v} + \mathbf{u}_b|^2 + 5(p_b + \Pi_b)\right](v_k + u_{bk})\right\} = P_b + M_b,
\end{aligned}
\tag{19}
$$

for $b = 1, \dots, n-1$. With this choice of governing equations, the vector of field variables becomes:

$$
\mathbf{u} = (\rho, \mathbf{v}, \varepsilon, \Pi, \rho_b, \mathbf{u}_b, \varepsilon_b, \Pi_b). \tag{20}
$$

2.3. Galilean Invariance

Rational extended thermodynamics postulates that the governing equations of the thermodynamic process have to be invariant with respect to Galilean transformation [42]. This condition is usually called the objectivity principle. To that end, we shall write the governing equations in a generic form:

$$
\frac{\partial}{\partial t}\mathbf{F}(\mathbf{u}) + \frac{\partial}{\partial x_k}\mathbf{F}_k(\mathbf{u}) = \mathbf{f}(\mathbf{u}); \quad \mathbf{F}_k(\mathbf{u}) = \mathbf{F}(\mathbf{u})v_k + \mathbf{\Phi}_k(\mathbf{u}), \tag{21}
$$

where $\mathbf{F}(\mathbf{u})$ is the vector of densities, $\mathbf{\Phi}_k(\mathbf{u})$ is the vector of non-convective fluxes, and $\mathbf{f}(\mathbf{u})$ is the vector of source (production) terms. If we represent the vector of field variables as $\mathbf{u} = (\mathbf{v}, \mathbf{w})$, where $\mathbf{w}$ is the vector of objective field variables, then Galilean invariance restricts the velocity dependence of densities, fluxes, and sources through the matrix $\mathbf{X}(\mathbf{v})$:

$$
\mathbf{F}(\mathbf{v}, \mathbf{w}) = \mathbf{X}(\mathbf{v})\hat{\mathbf{F}}(\mathbf{w}); \quad \mathbf{\Phi}_k(\mathbf{v}, \mathbf{w}) = \mathbf{X}(\mathbf{v})\hat{\mathbf{\Phi}}_k(\mathbf{w}); \quad \mathbf{f}(\mathbf{v}, \mathbf{w}) = \mathbf{X}(\mathbf{v})\hat{\mathbf{f}}(\mathbf{w}), \tag{22}
$$

where the hat denotes velocity-independent functions determined in the following way:

$$
\hat{\mathbf{F}}(\mathbf{w}) = \mathbf{F}(\mathbf{0}, \mathbf{w}); \quad \hat{\mathbf{\Phi}}_k(\mathbf{w}) = \mathbf{\Phi}_k(\mathbf{0}, \mathbf{w}); \quad \hat{\mathbf{f}}(\mathbf{w}) = \mathbf{f}(\mathbf{0}, \mathbf{w}),
$$

and $\mathbf{X}(\mathbf{0}) = \mathbf{I}$. From the governing Equations (18) and (19) one may deduce:

$$
\begin{aligned}
\mathbf{F}(\mathbf{v},\mathbf{w}) &= \begin{bmatrix} \rho \\ \rho v_i \\ \frac{1}{2}\rho|\mathbf{v}|^2 + \rho\varepsilon \\ \rho|\mathbf{v}|^2 + 3(p+\Pi) \\ \rho_b \\ \rho_b(v_i + u_{bi}) \\ \frac{1}{2}\rho_b|\mathbf{v}+\mathbf{u}_b|^2 + \rho_b\varepsilon_b \\ \rho_b|\mathbf{v}+\mathbf{u}_b|^2 + 3(p_b+\Pi_b) \end{bmatrix}; \\
\mathbf{\Phi}_k(\mathbf{v},\mathbf{w}) &= \begin{bmatrix} 0 \\ -t_{ik} \\ -t_{ki}v_i + q_k \\ 2(p+\Pi)v_k + 2v_l\hat{U}_{\langle lk\rangle} + \hat{F}_{llk} \\ \rho_b u_{bk} \\ \rho_b(v_i+u_{bi})u_{bk} + (p_b+\Pi_b)\delta_{ik} \\ \left(\frac{1}{2}\rho_b|\mathbf{v}+\mathbf{u}_b|^2 + \rho_b\varepsilon_b\right)u_{bk} + (p_b+\Pi_b)(v_k+u_{bk}) \\ \left[\rho_b|\mathbf{v}+\mathbf{u}_b|^2 + 3(p_b+\Pi_b)\right]u_{bk} + 2(p_b+\Pi_b)(v_k+u_{bk}) \end{bmatrix}; \\
\mathbf{f}(\mathbf{v},\mathbf{w}) &= \begin{bmatrix} 0 \\ 0_i \\ 0 \\ P \\ \tau_b \\ m_{bi} \\ e_b \\ P_b \end{bmatrix}.
\end{aligned}
\tag{23}
$$

The velocity transformation matrix then reads:

$$
\mathbf{X}(\mathbf{v}) = \begin{bmatrix}
1 & 0_k & 0 & 0 & 0 & 0_k & 0 & 0 \\
v_i & \delta_{ik} & 0_i & 0_i & 0_i & 0_{ik} & 0_i & 0_i \\
\frac{1}{2}|\mathbf{v}|^2 & v_k & 1 & 0 & 0 & 0_k & 0 & 0 \\
|\mathbf{v}|^2 & 2v_k & 0 & 1 & 0 & 0_k & 0 & 0 \\
0 & 0_k & 0 & 0 & 1 & 0_k & 0 & 0 \\
0_i & 0_{ik} & 0_i & 0_i & v_i & \delta_{ik} & 0_i & 0_i \\
0 & 0_k & 0 & 0 & \frac{1}{2}|\mathbf{v}|^2 & v_k & 1 & 0 \\
0 & 0_k & 0 & 0 & |\mathbf{v}|^2 & 2v_k & 0 & 1
\end{bmatrix}. \tag{24}
$$

Equation $(22)_{1,2}$ is identically satisfied by $(23)_{1,2}$ and (24), but $(22)_3$ restricts the velocity dependence of the source terms:

$$
\begin{aligned}
P &= \hat{P}; \\
\tau_b &= \hat{\tau}_b; \\
m_{bi} &= \hat{\tau}_b v_i + \hat{m}_{bi}; \\
e_b &= \frac{1}{2}\hat{\tau}_b|\mathbf{v}|^2 + \hat{m}_{bi}v_i + \hat{e}_b; \\
P_b + M_b &= \hat{P}_b + \hat{\tau}_b|\mathbf{v}|^2 + 2\hat{m}_{bi}v_i + \hat{M}_b.
\end{aligned}
\tag{25}
$$

2.4. Entropy Principle

The entropy inequality is a supplementary balance law in the form:

$$
\frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} = \Sigma \geq 0, \tag{26}
$$

where h, h_k, and Σ are the entropy density, the entropy flux, and the entropy production rate, respectively. These quantities may be expressed either in terms of $\tilde{\mathbf{u}} = (\mathbf{v}, \tilde{\mathbf{w}})$ (Equation (11)), or in terms of $\mathbf{u} = (\mathbf{v}, \mathbf{w})$ (Equation (20)). In either case, (26) must be invariant with respect to Galilean transformations, which yields:

$$h = h(\tilde{\mathbf{w}}),\ h_k = h_k(\tilde{\mathbf{w}}),\ \Sigma = \Sigma(\tilde{\mathbf{w}}) \quad \Leftrightarrow \quad h = h(\mathbf{w}),\ h_k = h_k(\mathbf{w}),\ \Sigma = \Sigma(\mathbf{w}).$$

Although both representations will be used in the sequel, we shall express the general results in terms of variables without a tilde, assuming that they are equally valid for the ones with a tilde.

The entropy principle, as formulated by Liu [43] and exploited in that way in ET, states that the entropy balance law (26) must be satisfied for any thermodynamic process governed by the balance laws (21). In this formulation governing equations are treated as constraints. Since governing equations and entropy balance law are both quasi-linear first-order partial differential equations, there exists a privileged (main) field $\mathbf{u}'(\mathbf{u})$ that acts as a vector of Lagrange multipliers, and secures compatibility between the master (entropy) equation and the constraints:

$$\frac{\partial h}{\partial t} + \frac{\partial h_k}{\partial x_k} - \Sigma = \mathbf{u}' \cdot \left(\frac{\partial \mathbf{F}}{\partial t} + \frac{\partial \mathbf{F}_k}{\partial x_k} - \mathbf{f} \right).$$

As a consequence, the following relations hold:

$$\mathrm{d}h = \mathbf{u}' \cdot \mathrm{d}\mathbf{F}, \quad \mathrm{d}h_k = \mathbf{u}' \cdot \mathrm{d}\mathbf{F}_k, \quad \Sigma = \mathbf{u}' \cdot \mathbf{f} \geq 0. \tag{27}$$

The systems of Equation $(27)_{1,2}$ serve to determine the main field and the entropy flux, which is a constitutive quantity. On the other hand, the residual inequality $(27)_3$ imposes restrictions on the structure of source terms.

The role of the main field is not exhausted with compatibility relations (27). In fact, if the entropy density h is a convex function of $\mathbf{F}$, then by means of Legendre transformation one may introduce the four potentials:

$$h' := \mathbf{u}' \cdot \mathbf{F} - h, \quad h'_k := \mathbf{u}' \cdot \mathbf{F}_k - h_k, \tag{28}$$

and transform the original system of balance laws (21) into symmetric hyperbolic form:

$$\frac{\partial}{\partial t}\left(\frac{\partial h'}{\partial \mathbf{u}'} \right) + \frac{\partial}{\partial x_k}\left(\frac{\partial h'_k}{\partial \mathbf{u}'} \right) = \mathbf{f} \quad \Leftrightarrow \quad \frac{\partial^2 h'}{\partial \mathbf{u}' \partial \mathbf{u}'} \frac{\partial \mathbf{u}'}{\partial t} + \frac{\partial^2 h'_k}{\partial \mathbf{u}' \partial \mathbf{u}'} \frac{\partial \mathbf{u}'}{\partial x_k} = \mathbf{f}. \tag{29}$$

Our aim is to apply these presented steps and apply the entropy principle to the mixture of polyatomic gases with dynamic pressure.

In particular, the entropy density of the mixture is defined as a sum of the entropy densities of the constituents:

$$h = \sum_{\alpha=1}^{n} (\rho_\alpha s_\alpha + \rho_\alpha k_\alpha), \tag{30}$$

where $s_\alpha(\rho_\alpha, \varepsilon_\alpha)$ is the partial equilibrium specific entropy, and $k_\alpha(\rho_\alpha, \varepsilon_\alpha, \Pi_\alpha)$ is the partial non-equilibrium specific entropy. This assumption restricts our study to the so-called simple mixtures. Denoting the main field components as:

$$\tilde{\mathbf{u}}' = (\tilde{\lambda}_\alpha, \tilde{\Lambda}_{\alpha i}, \tilde{\mu}_\alpha, \tilde{\zeta}_\alpha), \tag{31}$$

the compatibility condition $(27)_1$ may be expanded:

$$\begin{aligned}\mathrm{d}h = \sum_{\alpha=1}^{n} \mathrm{d}(\rho_\alpha s_\alpha + \rho_\alpha k_\alpha) = \sum_{\alpha=1}^{n} \Big\{ & \tilde{\lambda}_\alpha \mathrm{d}\rho_\alpha + \tilde{\Lambda}_{\alpha i} \mathrm{d}(\rho_\alpha v_{\alpha i}) \\ & + \tilde{\mu}_\alpha \mathrm{d}\left(\frac{1}{2}\rho_\alpha |\mathbf{v}_\alpha|^2 + \rho_\alpha \varepsilon_\alpha\right) + \tilde{\zeta}_\alpha \mathrm{d}\Big(\rho_\alpha |\mathbf{v}_\alpha|^2 + 3(p_\alpha + \Pi_\alpha)\Big)\Big\}.\end{aligned} \tag{32}$$

In the case of simple mixtures, (32) can be split into equations for the constituents, and straightforward calculation leads to the following main field:

$$\begin{aligned}\tilde{\lambda}_\alpha &= -\frac{1}{T_\alpha}\left(g_\alpha - \frac{1}{2}|\mathbf{v} + \mathbf{u}_\alpha|^2\right) - \left(\varepsilon_\alpha - \frac{1}{2}|\mathbf{v} + \mathbf{u}_\alpha|^2\right)\left(\frac{\partial k_\alpha}{\partial \varepsilon_\alpha} - \frac{\partial k_\alpha}{\partial \Pi_\alpha}\frac{\partial p_\alpha}{\partial \varepsilon_\alpha}\right) \\ &\quad - \rho_\alpha \frac{\partial k_\alpha}{\partial \Pi_\alpha}\left(\frac{\partial p_\alpha}{\partial \rho_\alpha} - \frac{1}{3}|\mathbf{v} + \mathbf{u}_\alpha|^2\right) + k_\alpha + \rho_\alpha \frac{\partial k_\alpha}{\partial \rho_\alpha}, \\ \tilde{\Lambda}_{\alpha i} &= -\frac{v_i + u_{\alpha i}}{T_\alpha} - \left(\frac{\partial k_\alpha}{\partial \varepsilon_\alpha} - \frac{\partial k_\alpha}{\partial \Pi_\alpha}\frac{\partial p_\alpha}{\partial \varepsilon_\alpha} + \frac{2}{3}\rho_\alpha \frac{\partial k_\alpha}{\partial \Pi_\alpha}\right)(v_i + u_{\alpha i}), \\ \tilde{\mu}_\alpha &= \frac{1}{T_\alpha} + \frac{\partial k_\alpha}{\partial \varepsilon_\alpha} - \frac{\partial k_\alpha}{\partial \Pi_\alpha}\frac{\partial p_\alpha}{\partial \varepsilon_\alpha}, \\ \tilde{\zeta}_\alpha &= \frac{1}{3}\rho_\alpha \frac{\partial k_\alpha}{\partial \Pi_\alpha}.\end{aligned} \tag{33}$$

Furthermore, it may be shown that dual entropy density has the form:

$$h' = -\sum_{\alpha=1}^{n}\left(\hat{\tilde{\mu}}_\alpha + 2\hat{\tilde{\zeta}}_\alpha\right)(p_\alpha + \Pi_\alpha) = \hat{h}'. \tag{34}$$

Finally, using $(28)_1$ in the form $\hat{h} = \hat{\tilde{\mathbf{u}}} \cdot \hat{\tilde{\mathbf{F}}} - \hat{h}'$, partial differential equations for non-equilibrium specific entropies are obtained:

$$\begin{aligned}&\rho_\alpha^2 \frac{\partial k_\alpha}{\partial \rho_\alpha} + (p_\alpha + \Pi_\alpha)\frac{\partial k_\alpha}{\partial \varepsilon_\alpha} \\ &\quad + \rho_\alpha\left\{-\rho_\alpha \frac{\partial p_\alpha}{\partial \rho_\alpha} + (p_\alpha + \Pi_\alpha)\left(\frac{5}{3} - \frac{1}{\rho_\alpha}\frac{\partial p_\alpha}{\partial \varepsilon_\alpha}\right)\right\}\frac{\partial k_\alpha}{\partial \Pi_\alpha} + \frac{\Pi_\alpha}{T_\alpha} = 0.\end{aligned} \tag{35}$$

It is obvious that Equation (35) for partial non-equilibrium specific entropies are not coupled, and have the same form (7) as the one in a single-component gas. Therefore, we may use the solution obtained in the ET6 case, and adapt it to the multi-component case:

$$k_\alpha = \frac{k_\mathrm{B}}{m_\alpha} \log\left\{X_\alpha^{3/2}\, Y_\alpha^{a_\alpha + 1}\right\}, \tag{36}$$

where m_α are the molecular masses of the constituents and

$$X_\alpha = 1 + \frac{\Pi_\alpha}{p_\alpha}, \quad Y_\alpha = 1 - \frac{3}{2(a_\alpha + 1)}\frac{\Pi_\alpha}{p_\alpha}. \tag{37}$$

The parameter $a_\alpha > -1$ can be related to the number of molecular degrees of freedom D_α of the constituent [20], $a_\alpha = (D_\alpha - 5)/2$, or to the specific heat [28].

Once the main field (33) and the non-equilibrium specific entropy are determined, the residual inequality may be exploited to determine the restrictions on the source terms. To that end, one has first to calculate the main field components with respect to **u** field variables (20). Denoting the main field components as:

$$\mathbf{u}' = (\lambda, \Lambda_i, \mu, \zeta, \lambda_b, \Lambda_{bi}, \mu_b, \zeta_b), \tag{38}$$

and using the density vector (23)$_1$, the compatibility condition (27)$_1$ becomes:

$$\begin{aligned}
\mathrm{d}h = {} & \lambda\,\mathrm{d}\rho + \Lambda_i\,\mathrm{d}(\rho\mathbf{v}) + \mu\,\mathrm{d}\left(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho\varepsilon\right) + \zeta\,\mathrm{d}\Big(\rho|\mathbf{v}|^2 + 3(p+\Pi)\Big) \\
& + \sum_{b=1}^{n-1}\{\lambda_b \mathrm{d}\rho_b + \Lambda_{bi}\mathrm{d}(\rho_b v_{bi}) \\
& + \mu_b \mathrm{d}\left(\frac{1}{2}\rho_b|\mathbf{v}_b|^2 + \rho_b\varepsilon_b\right) + \zeta_b \mathrm{d}\Big(\rho_b|\mathbf{v}_b|^2 + 3(p_b + \Pi_b)\Big)\Big\}.
\end{aligned} \tag{39}$$

Since dh must have the same form in (32) and (39), the following relations must hold:

$$\begin{aligned}
\lambda &= \tilde{\lambda}_n, & \lambda_b &= \tilde{\lambda}_b - \tilde{\lambda}_n, \\
\Lambda_i &= \tilde{\Lambda}_{ni}, & \Lambda_{bi} &= \tilde{\Lambda}_{bi} - \tilde{\Lambda}_{ni}, \\
\mu &= \tilde{\mu}_n, & \mu_b &= \tilde{\mu}_b - \tilde{\mu}_n, \\
\zeta &= \tilde{\zeta}_n, & \zeta_b &= \tilde{\zeta}_b - \tilde{\zeta}_n.
\end{aligned} \tag{40}$$

The explicit form of the main field is provided in Appendix A.

The residual inequality (27)$_3$ may be reduced to a velocity independent form:

$$\Sigma = \mathbf{u}' \cdot \mathbf{f} = \hat{\mathbf{u}}' \cdot \hat{\mathbf{f}} \geq 0,$$

which can be expanded to:

$$\Sigma = \hat{\zeta}\hat{P} + \sum_{b=1}^{n-1}\left\{\hat{\lambda}_b\hat{\tau}_b + \hat{\Lambda}_{bi}\hat{m}_{bi} + \hat{\mu}_b\hat{e}_b + \hat{\zeta}_b\big(\hat{P}_b + \hat{M}_b\big)\right\} \geq 0. \tag{41}$$

Taking into account identities $\hat{\zeta} = \tilde{\zeta}_n$ and $\hat{\zeta}_b + \tilde{\zeta}_n = \tilde{\zeta}_b$, as well as definition (13) of the source term in dynamic pressure balance laws for the mixture, (41) can be transformed into a linear combination of the source terms:

$$\Sigma = \sum_{\alpha=1}^{n}\tilde{\zeta}_\alpha\hat{P}_\alpha + \sum_{b=1}^{n-1}\left\{\hat{\lambda}_b\hat{\tau}_b + \hat{\Lambda}_{bi}\hat{m}_{bi} + \hat{\mu}_b\hat{e}_b + \hat{\zeta}_b\hat{M}_b\right\} \geq 0. \tag{42}$$

This equation imposes restrictions on the structure of source terms since the residual inequality (42) must be satisfied for any thermodynamic process.

The simplest possible way to secure the non-negativity of the entropy production rate (42) is to choose the source terms such that they become a positive semi-definite quadratic form. First, note that the internal dissipation terms $\hat{P}_\alpha$ are separated from the interaction terms. Taking into account that they are mutually independent functions of partial (constituent-related) objective quantities, one may choose them in the following form:

$$\hat{P}_\alpha = \omega_\alpha(\mathbf{w}_\alpha)\tilde{\zeta}_\alpha, \quad \alpha = 1, \ldots, n, \tag{43}$$

where $\omega_\alpha(\mathbf{w}_\alpha) \geq 0$, and $\mathbf{w}_\alpha$ denote the partial objective quantities. The remaining source terms may be constructed in the following way:

$$\begin{aligned}
\hat{\tau}_b &= \sum_{c=1}^{n-1} \Big(\varphi^\tau_{bc}(\mathbf{w})\hat{\lambda}_c + \varphi^e_{bc}(\mathbf{w})\hat{\mu}_c + \varphi^M_{bc}(\mathbf{w})\hat{\zeta}_c \Big), \\
\hat{m}_{bi} &= \sum_{c=1}^{n-1} \psi_{bc}(\mathbf{w})\hat{\Lambda}_{ci}, \\
\hat{e}_b &= \sum_{c=1}^{n-1} \Big(\theta^\tau_{bc}(\mathbf{w})\hat{\lambda}_c + \theta^e_{bc}(\mathbf{w})\hat{\mu}_c + \theta^M_{bc}(\mathbf{w})\hat{\zeta}_c \Big), \\
\hat{M}_b &= \sum_{c=1}^{n-1} \Big(\chi^\tau_{bc}(\mathbf{w})\hat{\lambda}_c + \chi^e_{bc}(\mathbf{w})\hat{\mu}_c + \chi^M_{bc}(\mathbf{w})\hat{\zeta}_c \Big).
\end{aligned} \tag{44}$$

Note that we took into account the cross-effects by expressing the source terms of the same tensorial order, here $\hat{\tau}_b$, $\hat{e}_b$, and $\hat{M}_b$, in terms of the main field components of the same order, i.e., $\hat{\lambda}_b$, $\hat{\mu}_b$, and $\hat{\zeta}_b$. This will be crucial for further matching of the macroscopic and the kinetic source terms, and explicit computation of the phenomenological coefficients, i.e., φs, ψs, θs, and χs. Furthermore, the phenomenological coefficients are matrix functions whose form must be such that quadratic form (42) is positive semi-definite.

In the sequel, we shall restrict the attention to chemically inert, i.e., non-reacting mixtures, which means that $\tau_\alpha = 0$ by assumption. As a consequence, $\varphi^\tau_{bc} = \varphi^e_{bc} = \varphi^M_{bc} = 0$, and $\theta^\tau_{bc} = \chi^\tau_{bc} = 0$.

2.5. Principal Subsystems of Non-Reacting Mixtures

The construction and properties of principal subsystems are exposed in detail in [44]. For their proper recognition, one has to analyze the system described by the main field $\mathbf{u}'$. Assume that the main field is split into two parts, $\mathbf{u}' = (\mathbf{v}', \mathbf{w}')$. Then, balance laws in symmetric form (29) may be written as:

$$\begin{aligned}
\frac{\partial}{\partial t}\left(\frac{\partial h'(\mathbf{v}', \mathbf{w}')}{\partial \mathbf{v}'} \right) + \frac{\partial}{\partial x_k}\left(\frac{\partial h'_k(\mathbf{v}', \mathbf{w}')}{\partial \mathbf{v}'} \right) &= \mathbf{p}(\mathbf{v}', \mathbf{w}'), \\
\frac{\partial}{\partial t}\left(\frac{\partial h'(\mathbf{v}', \mathbf{w}')}{\partial \mathbf{w}'} \right) + \frac{\partial}{\partial x_k}\left(\frac{\partial h'_k(\mathbf{v}', \mathbf{w}')}{\partial \mathbf{w}'} \right) &= \mathbf{r}(\mathbf{v}', \mathbf{w}').
\end{aligned}$$

The principal subsystem is the system obtained from the complete one when constant value $\mathbf{w}'_*$ is assigned to $\mathbf{w}'$:

$$\frac{\partial}{\partial t}\left(\frac{\partial h'(\mathbf{v}', \mathbf{w}'_*)}{\partial \mathbf{v}'} \right) + \frac{\partial}{\partial x_k}\left(\frac{\partial h'_k(\mathbf{v}', \mathbf{w}'_*)}{\partial \mathbf{v}'} \right) = \mathbf{p}(\mathbf{v}', \mathbf{w}'_*).$$

Such a subsystem is accompanied by a sub-entropy law for a properly defined sub-entropy, and its characteristic speeds satisfy the sub-characteristic condition—they are bounded by the characteristic speeds of the complete system restricted to the state space of the subsystem.

Restriction to the subsystem in terms of the main field amounts to discarding the balance laws in the original system to which $\mathbf{w}'$ corresponds. In most physically interesting cases, $\mathbf{w}'_* = \mathbf{0}$, since this part of the main field is usually related to non-equilibrium variables. In the sequel, we shall present the most important subsystems in the mixture of non-reacting polyatomic gases.

Case 1: Multi-temperature mixture of Euler fluids. First, the subsystem is obtained if we assume $\zeta_b = \tilde{\zeta}_b - \tilde{\zeta}_n = 0$, which immediately implies $\tilde{\zeta}_1 = \ldots = \tilde{\zeta}_n$, or explicitly:

$$\rho_1 \frac{\partial k_1}{\partial \Pi_1} = \ldots = \rho_n \frac{\partial k_n}{\partial \Pi_n} = C = \text{const}. \tag{45}$$

Constant C is common for all main fields since every k_α depends on the state variables of α constituent only. Although (45) indicates that every k_α is linear in Π_α, it is clear from (36) that conditions (45) cannot be satisfied unless $\Pi_\alpha / p_\alpha = 0$, i.e., $\Pi_\alpha = 0$ for all $\alpha = 1, \dots, n$. In such a way $C = 0$ and k_α is independent of Π_α, which implies that $k_\alpha(\rho_\alpha, \varepsilon_\alpha)$ becomes redundant and can be absorbed into $s_\alpha(\rho_\alpha, \varepsilon_\alpha)$. Therefore, we may take $k_\alpha = 0$, for all $\alpha = 1, \dots, n$, without the loss of generality.

A consequence of the result obtained under the assumption $\zeta_b = 0$ is that partial dynamic pressures vanish, and $\tilde{\zeta}_\alpha = 0$ and $\zeta = 0$. Therefore, in this subsystem, we may discard the balance laws $(19)_4$ for the dynamic pressure of the constituents, and the balance law $(18)_4$ for dynamic pressure of the mixture. Thus, we end up with the system $(18)_{1-3}$ and $(19)_{1-3}$, that is with the multi-temperature model for the mixture of Euler fluids, whose primal field variable vector is $\mathbf{u} = (\rho, \mathbf{v}, \varepsilon, \rho_b, \mathbf{u}_b, \varepsilon_b)$.

Case 2: Single-temperature mixture of Euler fluids. Next, a subsystem is obtained if, along with $\zeta_b = 0$, we assume $\mu_b = 0$. From the analysis of Case 1 we have $k_\alpha = 0$, so that condition $\mu_b = \tilde{\mu}_b - \tilde{\mu}_n = 0$ reduces to $T_1 = \ldots = T_n = T$. Therefore, we may discard the balance laws $(19)_3$ for the energy of the constituents, and we end up with a single-temperature model for the mixture of Euler fluids $(18)_{1-3}$ and $(19)_{1-2}$, whose primal field variable vector is $\mathbf{u} = (\rho, \mathbf{v}, \varepsilon, \rho_b, \mathbf{u}_b)$.

Case 3: Equilibrium subsystem. Among all principal subsystems, the equilibrium subsystem has a special status. It is the system for which the entropy production rate vanishes for all thermodynamic processes, $\Sigma_\mathrm{E} = 0$. In the case of a non-reacting mixture, this condition will be satisfied if and only if:

$$\hat{\zeta}_b = 0, \quad \hat{\tilde{\zeta}}_\alpha = 0, \quad \hat{\mu}_b = 0, \quad \hat{\Lambda}_{bi} = 0.$$

In Case 1 we saw that the first condition implies the second one; they imply $\Pi_\alpha = 0$ and $k_\alpha = 0$. Case 2, which corresponds to the third condition, imposed further restriction $T_\alpha = T$ for all the constituents. The last condition introduces the final restriction $u_{bi} = v_{bi} - v_i = 0$, i.e., $v_{\alpha i} = v_i$, which means that motion of all the constituents is described by the common velocity field. In that case, we may discard the balance laws $(19)_2$ for the momenta of constituents. The governing equations consist solely of balance laws $(18)_{1-3}$ and $(19)_1$, and the primal field variable vector is $\mathbf{u} = (\rho, \mathbf{v}, \varepsilon, \rho_b)$. To avoid ambiguity, we note that "equilibrium" does not mean that field variables are constant and uniform. The equilibrium subsystem rather defines an equilibrium manifold of the complete system on which the entropy production rate vanishes.

2.6. Linearized Source Terms in Non-Reacting Mixtures

Source terms (43) and (44) are expressed in terms of main field components and phenomenological coefficients. The macroscopic theory does not have means for the complete determination of the coefficients. However, they may be evaluated if the source terms obtained using the entropy principle are matched with the source terms obtained by the methods of kinetic theory. This matching cannot be performed in a general case, i.e., far from equilibrium, but only in the small neighborhood of the equilibrium manifold. To that end, we shall derive the linearized form of the source terms and use it in the sequel.

The equilibrium manifold, as determined in Case 3 of the previous Section, reads $\mathbf{u}_\mathrm{E} = (\rho, \mathbf{v}, \varepsilon, 0, \rho_b, \mathbf{0}, T, 0)$. The linearized form of the source terms (43) and (44) should be linear in $\mathbf{u} - \mathbf{u}_\mathrm{E}$. For $\hat{P}_\alpha$ we obtain from (36) and (43):

$$\hat{P}_\alpha^{\mathrm{lin}} = -\frac{1}{2} \frac{k_\mathrm{B}}{m_\alpha} \left(1 + \frac{3}{2(a_\alpha + 1)} \right) \omega_\alpha(\mathbf{w}_{\alpha\mathrm{E}}) \frac{\rho_\alpha}{p_{\alpha\mathrm{E}}^2} \Pi_\alpha, \tag{46}$$

where $\mathbf{w}_{\alpha\mathrm{E}}$ are partial objective quantities evaluated on the equilibrium manifold. For $\hat{m}_{bi}$, $\hat{e}_b$ and $\hat{M}_b$, from (36), (44), and (A3) we obtain:

$$\hat{m}_{bi}^{\mathrm{lin}} = -\sum_{c=1}^{n-1} \psi_{bc}(\mathbf{w}_\mathrm{E}) \frac{u_{ci} - u_{ni}}{T}, \tag{47}$$

$$\begin{aligned}
\hat{e}_b^{\mathrm{lin}} = \sum_{c=1}^{n-1} \theta_{bc}^{e}(\mathbf{w}_\mathrm{E}) \Bigg\{ & -\frac{\Theta_c - \Theta_n}{T^2} \\
& + \frac{3}{2}\frac{k_\mathrm{B}}{m_c}\left(1 + \frac{3}{2(a_c+1)}\right)\frac{\Pi_c}{p_{c\mathrm{E}}\varepsilon_{c\mathrm{E}}} - \frac{3}{2}\frac{k_\mathrm{B}}{m_n}\left(1 + \frac{3}{2(a_n+1)}\right)\frac{\Pi_n}{p_{n\mathrm{E}}\varepsilon_{n\mathrm{E}}} \Bigg\} \\
+ \sum_{c=1}^{n-1} \theta_{bc}^{M}(\mathbf{w}_\mathrm{E}) \Bigg\{ & -\frac{1}{2}\frac{k_\mathrm{B}}{m_c}\left(1 + \frac{3}{2(a_c+1)}\right)\frac{\rho_c}{p_{c\mathrm{E}}^2}\Pi_c \\
& + \frac{1}{2}\frac{k_\mathrm{B}}{m_n}\left(1 + \frac{3}{2(a_n+1)}\right)\frac{\rho_n}{p_{n\mathrm{E}}^2}\Pi_n \Bigg\},
\end{aligned} \tag{48}$$

$$\begin{aligned}
\hat{M}_b^{\mathrm{lin}} = \sum_{c=1}^{n-1} \chi_{bc}^{e}(\mathbf{w}_\mathrm{E}) \Bigg\{ & -\frac{\Theta_c - \Theta_n}{T^2} \\
& + \frac{3}{2}\frac{k_\mathrm{B}}{m_c}\left(1 + \frac{3}{2(a_c+1)}\right)\frac{\Pi_c}{p_{c\mathrm{E}}\varepsilon_{c\mathrm{E}}} - \frac{3}{2}\frac{k_\mathrm{B}}{m_n}\left(1 + \frac{3}{2(a_n+1)}\right)\frac{\Pi_n}{p_{n\mathrm{E}}\varepsilon_{n\mathrm{E}}} \Bigg\} \\
+ \sum_{c=1}^{n-1} \chi_{bc}^{M}(\mathbf{w}_\mathrm{E}) \Bigg\{ & -\frac{1}{2}\frac{k_\mathrm{B}}{m_c}\left(1 + \frac{3}{2(a_c+1)}\right)\frac{\rho_c}{p_{c\mathrm{E}}^2}\Pi_c \\
& + \frac{1}{2}\frac{k_\mathrm{B}}{m_n}\left(1 + \frac{3}{2(a_n+1)}\right)\frac{\rho_n}{p_{n\mathrm{E}}^2}\Pi_n \Bigg\},
\end{aligned} \tag{49}$$

where $u_{\alpha i} = v_{\alpha i} - v_i$ and $\Theta_\alpha = T_\alpha - T$. All the quantities with subscript E are evaluated on the equilibrium manifold. Although the coefficients are restricted to their values on the equilibrium manifold, it will turn out in the matching procedure that this is sufficient for the complete closure of the source terms and governing equations.

3. Kinetic Approach to the Mixture with Dynamic Pressure

A kinetic approach to the modeling of a polyatomic gas mixture will be based on the system of Boltzmann-like equations for a polyatomic gas mixture written in the so-called continuous internal energy setting. The model is introduced in [22,23] and assumes that the constituent α is described by a distribution function $f_\alpha = f_\alpha(t, \mathbf{x}, \boldsymbol{\xi}, I)$, which depends on macroscopic variables time $t \geq 0$ and space position $\mathbf{x}$, and on variables of microscopic nature, namely molecular velocity $\boldsymbol{\xi} \in \mathbb{R}^3$ and molecular continuous internal energy $I \in [0, \infty)$. If the distribution function changes due to transport and collisions between molecules, then its evolution can be modeled by the Boltzmann-like equation

$$\partial_t f_\alpha + \boldsymbol{\xi} \cdot \nabla_\mathbf{x} f_\alpha = \sum_{\beta=1}^{n} Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I). \tag{50}$$

The collision operator $Q_{\alpha\beta}(f_\alpha, f_\beta)$ encodes the influence of the constituent α on the constituent β due to molecular collisions, here assumed to be binary,

$$\begin{aligned}
& Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I) \\
& \quad = \int_{\Delta \times K} \left(f'_\alpha f'_{\beta*} \frac{I^{a_\alpha} I_*^{a_\beta}}{I'^{a_\alpha} I_*'^{a_\beta}} - f_\alpha f_{\beta*} \right) \mathcal{B}_{\alpha\beta}\, \psi_{\alpha\beta}(r, R)\, \mathrm{d}R\, \mathrm{d}r\, \mathrm{d}\sigma\, \mathrm{d}I_*\, \mathrm{d}\boldsymbol{\xi}_*,
\end{aligned} \tag{51}$$

for any $a_\alpha, a_\beta > -1$, with the region of integration

$$\Delta := \mathbb{R}^3 \times [0, +\infty), \quad K := [0,1]^2 \times S^2,$$

and standard abbreviations for a distribution function g,

$$g := g(t, \mathbf{x}, \boldsymbol{\xi}, I),\ g_* := g(t, \mathbf{x}, \boldsymbol{\xi}_*, I_*),\ g' := g(t, \mathbf{x}, \boldsymbol{\xi}', I'),\ g'_* := g(t, \mathbf{x}, \boldsymbol{\xi}'_*, I'_*).$$

The primed quantities corresponding to post-collisional velocity–internal energy pairs $(\boldsymbol{\xi}', I')$ and $(\boldsymbol{\xi}'_*, I'_*)$ are obtained from the pre-collisional ones using transformations

$$\begin{aligned} \boldsymbol{\xi}' &= \mathbf{G} + \frac{m_\beta}{m_\alpha + m_\beta}\sqrt{\frac{2RE}{\mu_{\alpha\beta}}}\sigma, & \boldsymbol{\xi}'_* &= \mathbf{G} - \frac{m_\alpha}{m_\alpha + m_\beta}\sqrt{\frac{2RE}{\mu_{\alpha\beta}}}\sigma, \\ I' &= r(1-R)E, & I'_* &= (1-r)(1-R)E, \end{aligned} \tag{52}$$

where the center-of-mass reference frame is introduced with the reduced mass $\mu_{\alpha\beta}$, velocity of the center of mass $\mathbf{G}$, and molecular relative velocity $\mathbf{g}$,

$$\mu_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}, \quad \mathbf{G} = \frac{m_\alpha \boldsymbol{\xi} + m_\beta \boldsymbol{\xi}_*}{m_\alpha + m_\beta}, \quad \mathbf{g} = \boldsymbol{\xi} - \boldsymbol{\xi}_*, \tag{53}$$

and the total energy of the molecular pair is

$$\frac{\mu_{\alpha\beta}}{2}|\mathbf{g}|^2 + I + I_* = \frac{\mu_{\alpha\beta}}{2}|\mathbf{g}'|^2 + I' + I'_* =: E. \tag{54}$$

Note that Equation (52) is a parametrization of the conservation laws at the collisional level

$$\begin{gathered} m_\alpha \boldsymbol{\xi} + m_\beta \boldsymbol{\xi}_* = m_\alpha \boldsymbol{\xi}' + m_\beta \boldsymbol{\xi}'_* \\ \frac{m_\alpha}{2}|\boldsymbol{\xi}|^2 + \frac{m_\beta}{2}|\boldsymbol{\xi}_*|^2 + I + I_* = \frac{m_\alpha}{2}|\boldsymbol{\xi}'|^2 + \frac{m_\beta}{2}|\boldsymbol{\xi}'_*|^2 + I' + I'_*, \end{gathered} \tag{55}$$

with the angular parameter $\sigma \in S^2$ (unit sphere in $\mathbb{R}^3$) and parameters of the Borgnakke–Larsen procedure $r, R \in [0,1]$.

The collision kernels $\mathcal{B}_{\alpha\beta} := \mathcal{B}_{\alpha\beta}(\boldsymbol{\xi}, \boldsymbol{\xi}_*, I, I_*, R, r, \sigma) \geq 0$ are assumed to be invariant with respect to collision transformations corresponding to the interchange of pre-post variables and the interchange of molecules, namely are assumed to satisfy the following two micro-reversibility assumptions

$$\begin{aligned} \mathcal{B}_{\alpha\beta} := \mathcal{B}_{\alpha\beta}(\boldsymbol{\xi}, \boldsymbol{\xi}_*, I, I_*, R, r, \sigma) &= \mathcal{B}_{\alpha\beta}(\boldsymbol{\xi}', \boldsymbol{\xi}'_*, I', I'_*, R', r', \sigma') \\ &= \mathcal{B}_{\beta\alpha}(\boldsymbol{\xi}_*, \boldsymbol{\xi}, I_*, I, R, 1-r, -\sigma). \end{aligned}$$

The function $\psi_{\alpha\beta}$ is defined by

$$\psi_{\alpha\beta}(r, R) = r^{a_\alpha}(1-r)^{a_\beta}(1-R)^{a_\alpha + a_\beta + 1}R^{1/2}. \tag{56}$$

It incorporates the Jacobian of the pre-post collision transformation [23,39] and its shape is a consequence of the choice of the gain term weight factor, both securing the well-defined collision operator weak form,

$$\begin{aligned} &\int_\Delta Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\chi(\boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi} \\ &\qquad = \int_{\Delta^2 \times K} (\chi' - \chi) f_\alpha\, f_{\beta *}\, \mathcal{B}_{\alpha\beta}\, \psi_{\alpha\beta}\, \mathrm{d}R\,\mathrm{d}r\,\mathrm{d}\sigma\,\mathrm{d}I_*\,\mathrm{d}\boldsymbol{\xi}_*\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}, \end{aligned} \tag{57}$$

for any suitable test function $\chi(\boldsymbol{\xi}, I)$. Note immediately that for the choice $\chi(\boldsymbol{\xi}, I) = m_\alpha$, the conservation property holds,

$$\int_\Delta m_\alpha \, Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi} = 0. \tag{58}$$

Another form can be obtained by taking test function $\phi(\boldsymbol{\xi}, I)$ and considering operators $Q_{\alpha\beta}$ and $Q_{\beta\alpha}$ simultaneously,

$$\begin{aligned}\int_\Delta \Big(Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\,\chi(\boldsymbol{\xi}, I) + Q_{\beta\alpha}(f_\beta, f_\alpha)(\boldsymbol{\xi}, I)\,\phi(\boldsymbol{\xi}, I)\Big)\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi} \\ = \int_{\Delta^2\times K} (\chi' + \phi'_* - \chi - \phi_*) f_\alpha\, f_{\beta *}\, \mathcal{B}_{\alpha\beta}\, \psi_{\alpha\beta}\, \mathrm{d}R\,\mathrm{d}r\,\mathrm{d}\sigma\,\mathrm{d}I_*\,\mathrm{d}\boldsymbol{\xi}_*\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}.\end{aligned}$$

It allows us to conclude that the conservation property for the test function corresponding to the molecule's momentum and energy is valid only for the same-species operator,

$$\int_\Delta \begin{pmatrix} m_\alpha \boldsymbol{\xi} \\ \frac{m_\alpha}{2}|\boldsymbol{\xi}|^2 + I \end{pmatrix} Q_{\alpha\alpha}(f_\alpha, f_\alpha)(\boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi} = 0.$$

Otherwise, interactions with different constituents induce non-vanishing collision operators and production terms for the right-hand side of (50) when appropriately integrated. Conservation property holds only for the whole mixture, i.e.,

$$\sum_{\alpha=1}^{n} \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{n} \int_\Delta \begin{pmatrix} m_\alpha \boldsymbol{\xi} \\ \frac{m_\alpha}{2}|\boldsymbol{\xi}|^2 + I \end{pmatrix} Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi} = 0.$$

Furthermore, for models (50) and (51), the H-theorem is proved in [22,23] with the entropy production D defined as

$$D = \sum_{\alpha,\beta=1}^{n} \int_\Delta Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\, \log\!\big(f_\alpha(\boldsymbol{\xi}, I) I^{-a_\alpha}\big)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}, \tag{59}$$

and the equilibrium distribution function

$$f_\alpha(\boldsymbol{\xi}, I) = \frac{\rho_\alpha}{m_\alpha} \frac{I^{a_\alpha}}{(k_B T)^{a_\alpha+1}\Gamma(a_\alpha+1)} \left(\frac{m_\alpha}{2\pi k_B T}\right)^{\frac{3}{2}} e^{-\frac{1}{k_B T}\left(\frac{m_\alpha}{2}|\boldsymbol{\xi}-\boldsymbol{v}|^2 + I\right)}, \tag{60}$$

with $\rho_\alpha, T > 0$ and $\boldsymbol{v} \in \mathbb{R}^3$, where Γ represents the Gamma function.

3.1. Macroscopic Densities as Moments of the Distribution Function

The six-moment macroscopic model (9) can be obtained starting from the Boltzmann Equation (50) by integration against the suitable test functions over the space of microscopic variables $(\boldsymbol{\xi}, I) \in \Delta = \mathbb{R}^3 \times [0, \infty)$. Test functions that correspond to the six-moment models are

$$m_\alpha, \quad m_\alpha \boldsymbol{\xi}, \quad \frac{m_\alpha}{2}|\boldsymbol{\xi}|^2 + I, \quad m_\alpha |\boldsymbol{\xi}|^2. \tag{61}$$

In order to define each macroscopic density appearing in (9) as the moment of the distribution function f_α we first introduce the peculiar velocity $\mathbf{c}_\alpha$ as the relative velocity of the molecule with respect to the macroscopic velocity $\boldsymbol{v}_\alpha$ of the constituent α,

$$\mathbf{c}_\alpha = \boldsymbol{\xi} - \boldsymbol{v}_\alpha. \tag{62}$$

Then, the macroscopic densities are defined as follows

$$\begin{pmatrix} \rho_\alpha \\ \rho_\alpha v_\alpha \\ \rho_\alpha \varepsilon_\alpha \\ 3(p_\alpha + \Pi_\alpha) \end{pmatrix} = \int_\Delta \begin{pmatrix} m_\alpha \\ m_\alpha \boldsymbol{\xi} \\ \frac{m_\alpha}{2}|\mathbf{c}_\alpha|^2 + I \\ m_\alpha |\mathbf{c}_\alpha|^2 \end{pmatrix} f_\alpha(t, x, \boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}, \tag{63}$$

corresponding to the mass, momentum, and total energy density and the trace of the momentum flux for α-th component of the gas. Moreover, entropy densities of the constituents (30) can be defined as the moment of the distribution function as well,

$$h_\alpha = -k_B \int_\Delta f_\alpha \, \log(f_\alpha I^{-a_\alpha})\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}. \tag{64}$$

Since in this paper we restrict attention to polyatomic ideal gases with constant specific heats, we use the following relations throughout the paper,

$$p_\alpha = \frac{\rho_\alpha}{m_\alpha} k_B T_\alpha, \qquad \varepsilon_\alpha = \left(a_\alpha + \tfrac{5}{2}\right)\frac{p_\alpha}{\rho_\alpha}, \tag{65}$$

for any constituent $\alpha = 1, \ldots, n$.

3.2. Macroscopic Equations as Moments of the Boltzmann Equation

The governing equations for densities (63) can be derived from the kinetic theory by means of the integration of the Boltzmann equation (50) against the six test functions (61). These evolution equations correspond to the ones from extended thermodynamics (9) after we define the non-convective fluxes,

$$\begin{pmatrix} t_{\alpha ik} \\ q_{\alpha k} \\ F_{\alpha \ell \ell k} \end{pmatrix} = \int_\Delta \begin{pmatrix} -m_\alpha c_{\alpha i} c_{\alpha k} \\ \left(\frac{m_\alpha}{2}|\mathbf{c}_\alpha|^2 + I\right) c_{\alpha k} \\ m_\alpha |\mathbf{c}_\alpha|^2 \, c_{\alpha k} \end{pmatrix} f_\alpha(t, x, \boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}, \tag{66}$$

as much as the production terms corresponding to the momentum and energy density and trace of the momentum flux equation, respectively,

$$\begin{pmatrix} \mathfrak{m}_\alpha \\ \mathfrak{e}_\alpha \\ \mathfrak{P}_\alpha \end{pmatrix} = \sum_\beta \int_\Delta \begin{pmatrix} m_\alpha \boldsymbol{\xi} \\ \frac{m_\alpha}{2}|\boldsymbol{\xi}|^2 + I \\ m_\alpha |\boldsymbol{\xi}|^2 \end{pmatrix} Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}. \tag{67}$$

We immediately realize

$$\mathfrak{e}_\alpha = \frac{1}{2}\mathfrak{P}_\alpha + \tilde{\mathfrak{e}}_\alpha, \text{ where } \quad \tilde{\mathfrak{e}}_\alpha = \sum_\beta \int_\Delta I \, Q_{\alpha\beta}(f_\alpha, f_\beta)(\boldsymbol{\xi}, I)\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi}. \tag{68}$$

Note that for the production term τ_α from (9) it holds $\tau_\alpha = 0$ in this model, because of the weak form conservative property (58).

3.3. Maximum Entropy Principle for the Six-Field Mixture Model

The aim of this section is to formulate the maximum entropy principle (MEP) with the constraints corresponding to the macroscopic densities (63). The outcome of this principle is the distribution function whose dependence on the variables t, x is through the densities (63). We will show in the upcoming Section 3.4 that such a distribution function yields the closure of fluxes (66) since it enables expressing these fluxes in terms of densities, as much as the computation of the production terms (67), for the specific choice of the collision kernel.

Lemma 1 (**Six-field distribution function**)**.** *Solution of the maximum entropy principle*

$$
\begin{aligned}
&max_{(f_1,\ldots,f_n)} \quad h = -k_B \sum_{\alpha=1}^{n} \int_\Delta f_\alpha \, \log(f_\alpha I^{-a_\alpha}) \, \mathrm{d}I \, \mathrm{d}\boldsymbol{\xi} \\
&s.t. \begin{pmatrix} \rho_\alpha \\ 0 \\ \left(a_\alpha + \frac{5}{2}\right) p_\alpha \\ 3(p_\alpha + \Pi_\alpha) \end{pmatrix} = \int_\Delta \begin{pmatrix} m_\alpha \\ m_\alpha \mathbf{c}_\alpha \\ \frac{m_\alpha}{2} |\mathbf{c}_\alpha|^2 + I \\ m_\alpha |\mathbf{c}_\alpha|^2 \end{pmatrix} f_\alpha \, \mathrm{d}I \, \mathrm{d}\boldsymbol{\xi}.
\end{aligned}
\tag{69}
$$

for any $\alpha = 1, \ldots, n$ is given with

$$
\hat{f}^6_\alpha = I^{a_\alpha} \frac{\rho_\alpha}{m_\alpha} \left(\frac{U_\alpha}{\pi}\right)^{\frac{3}{2}} \frac{V_\alpha^{a_\alpha+1}}{\Gamma(a_\alpha+1)} e^{-\left(U_\alpha |\boldsymbol{\xi} - \mathbf{v}_\alpha|^2 + V_\alpha I\right)},
\tag{70}
$$

$$
U_\alpha = \frac{m_\alpha}{2kT_\alpha} X_\alpha^{-1}, \qquad V_\alpha = \frac{1}{kT_\alpha} Y_\alpha^{-1},
\tag{71}
$$

with X_α and Y_α from (37), that provides convergent moments if $X_\alpha > 0$ and $Y_\alpha > 0$.

We refer to (70) as the six-field distribution function.

Proof. The extended functional for this variational problem with constraints is

$$
\begin{aligned}
\mathcal{L} = h - \tilde{\lambda}_\alpha \int_\Delta m_\alpha f_\alpha \, \mathrm{d}I \, \mathrm{d}\boldsymbol{\xi} + \tilde{\Lambda}_{\alpha i} \int_\Delta m_\alpha c_{\alpha i} f_\alpha \, \mathrm{d}I \, \mathrm{d}\boldsymbol{\xi} \\
+ \tilde{\mu}_\alpha \int_\Delta \left(\frac{m_\alpha}{2} |\mathbf{c}_\alpha|^2 + I\right) f_\alpha \, \mathrm{d}I \, \mathrm{d}\boldsymbol{\xi} + \tilde{\zeta}_\alpha \int_\Delta m_\alpha |\mathbf{c}_\alpha|^2 f_\alpha \, \mathrm{d}I \, \mathrm{d}\boldsymbol{\xi},
\end{aligned}
\tag{72}
$$

where $\tilde{\lambda}_\alpha$, $\tilde{\Lambda}_{\alpha i}$, $\tilde{\mu}_\alpha$, and $\tilde{\zeta}_\alpha$ are multipliers that coincide with the ones from (32), and we have used the summation convention (10). The Euler–Lagrange equation reduces to $\delta \mathcal{L} / \delta f_\alpha = 0$, whose solution is

$$
\hat{f}_\alpha = I^{a_\alpha} e^{-1 - \frac{m_\alpha}{k_B} \tilde{\lambda}_\alpha - \frac{m_\alpha}{k_B} \tilde{\Lambda}_{\alpha i} c_{\alpha i} - \frac{1}{k_B} \tilde{\mu}_\alpha \left(\frac{m_\alpha}{2} |\mathbf{c}_\alpha|^2 + I\right) - \frac{m_\alpha}{k_B} \tilde{\zeta}_\alpha |\mathbf{c}_\alpha|^2}.
$$

We plug this distribution function into constraints of the problem (69), which allows expressing multipliers in terms of macroscopic densities, which yields the final expression $\hat{f}^6_\alpha$ as in (70). ☐

The six-field distribution function (70) yields the closure of the six-field model for a polyatomic gas mixture (9), as shown in the upcoming Section 3.4.

3.4. Closure of the 6-Moment Mixture Model

In this section, we start with the six-field distribution function (70) and plug it into the definition of the unknown non-convective fluxes (66) and the production terms (67) for a specific choice of the collision kernel, that will allow the closure of the system (9).

Taking $f = \hat{f}^6_\alpha$ in (66), by exploiting parity arguments we obtain the following expressions for the non-convective fluxes,

$$
t_{\alpha ik} = (p_\alpha + \Pi_\alpha) \delta_{ik}, \qquad q_{\alpha k} = 0, \qquad F_{\alpha \ell \ell k} = 0.
$$

Therefore, we conclude that the approach from the kinetic theory yields the same left-hand side expressions as the model issuing from the extended thermodynamics described in (9).

Next, our aim is to compute production terms $\mathfrak{m}_\alpha$, $\mathfrak{e}_\alpha$ and $\mathfrak{P}_\alpha$ that correspond to the balance law of momentum and energy density and momentum flux for each species α, $\alpha = 1, \ldots, n$, as defined in (67). Production terms can be determined only for a specific choice of the collision kernel. In this manuscript, we take the collision kernel model recently proposed in the study of the well-posedness of the space homogeneous system of Boltzmann equations describing a mixture of monatomic and polyatomic gases [39]. The same form in the case of single polyatomic gas with frozen collisions was already shown to be consistent with the experimental data and DSMC method in the series of papers [28–30]. Moreover, in the case of the six-moment model for a single polyatomic gas in [27], it is shown that such a collision kernel model provides complete agreement with extended thermodynamics models of six fields [32], as it satisfies the entropy residual inequality on the whole range of model validity.

Thus, we take the following collision kernel model

$$\begin{aligned}&\mathcal{B}_{\alpha\beta}(\boldsymbol{\xi},\boldsymbol{\xi}_*,I,I_*,R,r,\sigma)\\&\quad=K_{\alpha\beta}\,k_{\alpha\beta}\left(\left(R|\boldsymbol{\xi}-\boldsymbol{\xi}_*|^2\right)^{\frac{\gamma_{\alpha\beta}}{2}}+\eta\left(\frac{r(1-R)I}{\sum_\alpha m_\alpha}\right)^{\frac{\gamma_{\alpha\beta}}{2}}+\eta\left(\frac{(1-r)(1-R)I_*}{\sum_\alpha m_\alpha}\right)^{\frac{\gamma_{\alpha\beta}}{2}}\right),\end{aligned}\tag{73}$$

where $K_{\alpha\beta} = K_{\beta\alpha} > 0$ is the dimensional constant, the constant $k_{\alpha\beta}$ serves to achieve consistency with the monatomic case [29],

$$k_{\alpha\beta}=\frac{2}{\sqrt{\pi}}\frac{\Gamma(a_\alpha+a_\beta+\frac{7}{2})}{\Gamma(a_\alpha+1)\Gamma(a_\beta+1)},\tag{74}$$

$\gamma_{\alpha\beta} = \gamma_{\beta\alpha} \geq 0$ is the potential rate and $\eta > 0$ controls the influence of the internal energy.

Production terms are computed in the Appendix C, here we only summarize the final result. Let us introduce constants

$$\begin{aligned}\mathcal{K}_{\alpha\beta}&=K_{\alpha\beta}\frac{1}{m_\alpha m_\beta}8\sqrt{\pi}\frac{\Gamma(a_\alpha+a_\beta+\frac{7}{2})}{\Gamma(a_\alpha+a_\beta+\frac{\gamma_{\alpha\beta}+9}{2})},\\\mathcal{C}_\iota&=\frac{\Gamma\left(a_\iota+1+\frac{\gamma_{\alpha\beta}}{2}\right)^2}{\Gamma(a_\iota+1)^2}\frac{\sqrt{\pi}}{2}\left(\sum_\alpha m_\alpha\right)^{-\gamma_{\alpha\beta}/2},\quad\text{for }\iota=\alpha,\beta,\end{aligned}\tag{75}$$

and terms involving regularized hypergeometric functions defined in (A6),

$$\begin{aligned}\mathcal{F}^1_y&=e^{-a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2}a_{\alpha\beta}^{-y/2}\,\Gamma\left(\tfrac{y+3}{2}\right)\,{}_1\tilde{F}_1\left(\tfrac{y+3}{2},\tfrac{3}{2},a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2\right),\\\mathcal{F}^2_y&=e^{-a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2}a_{\alpha\beta}^{-y/2}\,\Gamma\left(\tfrac{y+5}{2}\right)\,{}_1\tilde{F}_1\left(\tfrac{y+5}{2},\tfrac{5}{2},a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2\right),\end{aligned}\tag{76}$$

for some $y \geq 0$, with

$$a_{\alpha\beta}=\frac{U_\alpha U_\beta}{U_\alpha+U_\beta},\tag{77}$$

for U_α and U_β defined in (71), and the term

$$D_{\alpha\beta}=-\frac{m_\beta}{m_\alpha+m_\beta}(a_\alpha+a_\beta+2)+2\frac{\mu_{\alpha\beta}}{(U_\alpha+U_\beta)}\left(\frac{U_\alpha}{m_\alpha}-\frac{U_\beta}{m_\beta}\right)\left(a_\alpha+a_\beta+\tfrac{\gamma_{\alpha\beta}+7}{2}\right).$$

The source term corresponding to the momentum of the constituent α is

$$
\begin{aligned}
\mathfrak{m}_\alpha &= \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{n} \rho_\alpha\rho_\beta\, \mathcal{K}_{\alpha\beta}\, \mathfrak{m}_{\alpha\beta} \\
&= -\sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{n} \rho_\alpha\rho_\beta\, \mathcal{K}_{\alpha\beta} (\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta)\, \mu_{\alpha\beta} \Big(a_\alpha + a_\beta + \tfrac{\gamma_{\alpha\beta}+7}{2}\Big) \\
&\quad \times \left(\Gamma(\tfrac{3+\gamma_{\alpha\beta}}{2})\mathcal{F}^2_{\gamma_{\alpha\beta}} + \eta\left(\frac{\mathcal{C}_\alpha}{V_\alpha^{\gamma_{\alpha\beta}/2}} + \frac{\mathcal{C}_\beta}{V_\beta^{\gamma_{\alpha\beta}/2}}\right)\right),
\end{aligned} \tag{78}
$$

with V_α and V_β defined in (71).

The source term $\mathfrak{P}_\alpha$ in the equation for dynamical pressure of the constituent α has a part related to the source term $\mathfrak{m}_\alpha$ and the internal part $\tilde{\mathfrak{P}}_\alpha$,

$$
\begin{aligned}
\mathfrak{P}_\alpha &= \tilde{\mathfrak{P}}_\alpha + 2\sum_{\beta=1}^{n} \frac{U_\alpha \boldsymbol{v}_\alpha + U_\beta \boldsymbol{v}_\beta}{U_\alpha + U_\beta} \cdot (\rho_\alpha\rho_\beta\mathcal{K}_{\alpha\beta}\mathfrak{m}_{\alpha\beta}) \\
&= \sum_{\beta=1}^{n} \rho_\alpha\rho_\beta\mathcal{K}_{\alpha\beta}\left(\tilde{\mathfrak{P}}_{\alpha\beta} + 2\frac{U_\alpha \boldsymbol{v}_\alpha + U_\beta \boldsymbol{v}_\beta}{U_\alpha + U_\beta} \cdot \mathfrak{m}_{\alpha\beta}\right) \\
&= \sum_{\beta=1}^{n} \rho_\alpha\rho_\beta\mathcal{K}_{\alpha\beta}\mathfrak{P}_{\alpha\beta},
\end{aligned} \tag{79}
$$

where the internal part $\tilde{\mathfrak{P}}_{\alpha\beta}$ reads

$$
\begin{aligned}
\tilde{\mathfrak{P}}_{\alpha\beta} &= \mu_{\alpha\beta} D_{\alpha\beta} \Gamma\Big(\tfrac{\gamma_{\alpha\beta}+3}{2}\Big) \mathcal{F}^1_{2+\gamma_{\alpha\beta}} \\
&\quad + \frac{2\,m_\beta}{m_\alpha + m_\beta} \Gamma\Big(\tfrac{\gamma_{\alpha\beta}+5}{2}\Big) \left(\frac{a_\alpha + 1}{V_\alpha} + \frac{a_\beta + 1}{V_\beta}\right) \mathcal{F}^1_{\gamma_{\alpha\beta}} \\
&\quad + \eta\, \mu_{\alpha\beta} \left(D_{\alpha\beta} - \frac{m_\beta}{m_\alpha + m_\beta}\frac{\gamma_{\alpha\beta}}{2}\right) \left(\frac{\mathcal{C}_\alpha}{N_\alpha^{\gamma_{\alpha\beta}/2}} + \frac{\mathcal{C}_\beta}{N_\beta^{\gamma_{\alpha\beta}/2}}\right) \mathcal{F}^1_2 \\
&\quad + 3\eta \frac{m_\beta}{m_\alpha + m_\beta} \left(\left(\frac{a_\alpha + 1 + \frac{\gamma_{\alpha\beta}}{2}}{V_\alpha} + \frac{a_\beta + 1}{V_\beta} \right) \frac{\mathcal{C}_\alpha}{V_\alpha^{\gamma_{\alpha\beta}/2}} \right. \\
&\quad \left. + \left(\frac{a_\beta + 1 + \frac{\gamma_{\alpha\beta}}{2}}{V_\beta} + \frac{a_\alpha + 1}{V_\alpha} \right) \frac{\mathcal{C}_\beta}{V_\beta^{\gamma_{\alpha\beta}/2}} \right).
\end{aligned} \tag{80}
$$

Note that the part containing $\mathfrak{m}_{\alpha\beta}$ vanishes when summed over α because it changes the sign when α is interchanged with β, i.e., $\mathfrak{m}_{\alpha\beta} = -\mathfrak{m}_{\beta\alpha}$, implying

$$
2\sum_{\alpha=1}^{n} \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{n} \rho_\alpha\rho_\beta\, \mathcal{K}_{\alpha\beta} \left(\frac{U_\alpha \boldsymbol{v}_\alpha + U_\beta \boldsymbol{v}_\beta}{U_\alpha + U_\beta}\right) \cdot \mathfrak{m}_{\alpha\beta} = 0,
$$

Thus, this part can be included in the interaction source term M_α from (9) obtained within extended thermodynamics modeling.

Finally, the production term in the balance law for the total energy of the constituent α is determined by (68)

$$\mathfrak{e}_\alpha = \frac{1}{2}\mathfrak{P}_\alpha + \tilde{\mathfrak{e}}_\alpha = \sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n} \rho_\alpha\rho_\beta\,\mathcal{K}_{\alpha\beta}\left(\frac{\mathfrak{P}_{\alpha\beta}}{2} + \tilde{\mathfrak{e}}_{\alpha\beta}\right),$$

with $\tilde{\mathfrak{e}}_{\alpha\beta}$ given by

$$\begin{aligned}
\tilde{\mathfrak{e}}_{\alpha\beta} = {}& (a_\alpha+1)\Gamma\Big(\tfrac{\gamma_{\alpha\beta}+3}{2}\Big) \\
& \times \left\{ \frac{\mu_{\alpha\beta}}{2}\mathcal{F}^1_{2+\gamma_{\alpha\beta}} + \left((a_\beta+1)\left(\frac{1}{V_\beta} - \frac{1}{V_\alpha}\right) - \frac{\frac{\gamma_{\alpha\beta}}{2} + \frac{3}{2}}{V_\alpha} \right)\mathcal{F}^1_{\gamma_{\alpha\beta}} \right\} \\
& + \eta\,\frac{\mu_{\alpha\beta}}{2}\left(\frac{a_\alpha + 1 + \frac{\gamma_{\alpha\beta}}{2}}{V_\alpha^{\gamma_{\alpha\beta}/2}}\mathcal{C}_\alpha + \frac{a_\alpha+1}{V_\beta^{\gamma_{\alpha\beta}/2}}\mathcal{C}_\beta \right)\mathcal{F}^1_2 \\
& + \eta\Big(a_\alpha + 1 + \tfrac{\gamma_{\alpha\beta}}{2}\Big)\frac{\mathcal{C}_\alpha}{V_\alpha^{\gamma_{\alpha\beta}/2}}\left(\frac{a_\beta+1}{V_\beta} - \frac{a_\beta + \frac{5}{2}}{V_\alpha} \right) \\
& + \eta(a_\alpha+1)\frac{\mathcal{C}_\beta}{V_\beta^{\gamma_{\alpha\beta}/2}}\left(\frac{a_\beta + 1 + \frac{\gamma_{\alpha\beta}}{2}}{V_\beta} - \frac{a_\beta + \frac{5}{2} + \frac{\gamma_{\alpha\beta}}{2}}{V_\alpha} \right).
\end{aligned} \tag{81}$$

3.5. *Linearized Source Terms in the Kinetic Approach*

We introduce the following shorthand notation,

$$w = \big(\boldsymbol{v}_\alpha, \boldsymbol{v}_\beta, T_\alpha, T_\beta, \Pi_\alpha, \Pi_\beta\big), \quad w^0 = (\boldsymbol{v}, \boldsymbol{v}, T, T, 0, 0).$$

For a production term $\mathcal{A} = \mathcal{A}(w)$, which in general depends on the vector of variables w, the linearization is obtained via

$$\mathcal{A}(w) \approx \mathcal{A}(w^0) + \nabla\mathcal{A}(w^0)\cdot\Big(w - w^0\Big) =: \mathcal{A}^{\text{lin}}.$$

In the present paper, we consider production terms $\mathfrak{m}_\alpha$, $\mathfrak{P}_\alpha$ and $\mathfrak{e}_\alpha$ corresponding to the momentum, non-equilibrium pressure, and internal energy production terms that are computed in (78), (80) with (79), and (81) with (68), respectively. First, we observe that all of them vanish at the equilibrium state,

$$\mathfrak{m}_\alpha(w^0) = 0, \quad \mathfrak{P}_\alpha(w^0) = 0 \quad \text{and} \quad \mathfrak{e}_\alpha(w^0) = 0.$$

Then it is needed to compute gradients. Computations are performed in Appendix D, here we only list the final results.

The production term $\mathfrak{m}_\alpha$ is approximated as follows

$$\mathfrak{m}_\alpha^{\text{lin}} = -\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n} \rho_\alpha\rho_\beta\,\mathcal{M}_{\alpha\beta}\,T^{\frac{\gamma_{\alpha\beta}}{2}}\,(\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta), \tag{82}$$

where the constant $\mathcal{M}_{\alpha\beta} \geq 0$ is symmetric in (α, β), whose form is detailed in (A23).

The production term $\mathfrak{P}_\alpha$ given in (79) is linearized as follows

$$\begin{aligned}
\mathfrak{P}_\alpha^{\text{lin}} = {}& 2\,\boldsymbol{v}\cdot\mathfrak{m}_\alpha^{\text{lin}} \\
& - \sum_{\beta=1}^{n} \rho_\alpha\rho_\beta\left(\mathcal{P}^T_{\alpha\beta}\,T^{\frac{\gamma_{\alpha\beta}}{2}}\,(T_\alpha - T_\beta) + \mathcal{P}^\Pi_{\alpha\beta}\,T^{\frac{\gamma_{\alpha\beta}}{2}}\,\frac{\Pi_\alpha}{k_B\,n_\alpha} - \tilde{\mathcal{P}}^\Pi_{\alpha\beta}\,T^{\frac{\gamma_{\alpha\beta}}{2}}\,\frac{\Pi_\beta}{k_B\,n_\beta} \right),
\end{aligned} \tag{83}$$

where $\mathcal{P}^{T}_{\alpha\beta} > 0$, $\mathcal{P}^{\Pi}_{\alpha\beta} > 0$ and $\tilde{\mathcal{P}}^{\Pi}_{\alpha\beta}$ are constants listed in (A25) that do not experience any symmetry in (α, β).

The production term $\mathfrak{e}_{\alpha}$ is linearized as follows

$$\begin{aligned} \mathfrak{e}^{\text{lin}}_{\alpha} &= \boldsymbol{v} \cdot \mathfrak{m}^{\text{lin}}_{\alpha} \\ &\quad - \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{n} \rho_{\alpha}\rho_{\beta} \left(\mathcal{E}^{T}_{\alpha\beta}\, T^{\frac{\gamma_{\alpha\beta}}{2}} (T_{\alpha} - T_{\beta}) - \mathcal{E}^{\Pi}_{\alpha\beta}\, T^{\frac{\gamma_{\alpha\beta}}{2}} \frac{\Pi_{\alpha}}{k_B\, n_{\alpha}} + \mathcal{E}^{\Pi}_{\beta\alpha}\, T^{\frac{\gamma_{\alpha\beta}}{2}} \frac{\Pi_{\beta}}{k_B\, n_{\beta}} \right), \end{aligned} \quad (84)$$

where the term $\mathfrak{m}^{\text{lin}}_{\alpha}$ is from (82), $\mathcal{E}^{T}_{\alpha\beta} > 0$ and $\mathcal{E}^{\Pi}_{\alpha\beta}$ are explicitly given in (A31). Let us emphasize that $\mathcal{E}^{T}_{\alpha\beta}$ is positive and symmetric in (α, β).

4. Macroscopic/Kinetic Closure

It is shown in previous sections that the macroscopic approach of extended thermodynamics and kinetic approach based upon moment equations lead to almost equivalent models of gaseous mixtures with dynamic pressure. In fact, the differential part of RET governing Equation (9) is the same as the differential part of the moment equations derived in the kinetic approach (see Section 3.2). The difference lies in the functional form of the source terms. Although the RET source terms have a form that nicely reflects their interaction character, they have one shortcoming—phenomenological coefficients cannot be completely determined within this framework. On the other, within the chosen level of approximation (determined by MEP), the kinetic source terms can be explicitly computed and expressed in terms of macroscopic field variables and properties of the constituents. However, their functional form is less appreciable than the one of extended thermodynamics.

To keep the advantages of both approaches we propose a combined macroscopic/kinetic closure. It is based upon the fact that either source terms have the same form of linear approximation in the neighborhood of the equilibrium manifold. Therefore, we may use the kinetic source terms in the linearized form to determine the phenomenological coefficients of the macroscopic source terms. This method has already been applied to a multi-temperature mixture of Euler fluids [40]. Although these coefficients will be computed on an equilibrium manifold, they present a first approximation of the general phenomenological coefficients. Thus, they can be plugged back into nonlinear source terms of extended thermodynamics. In such a way, the nonlinear part of the source terms will still bring the desired information about the non-equilibrium behavior of the system. This was recently used in the analysis of shock structure in multi-component mixtures [13,41].

In the sequel, the phenomenological coefficients will be computed for each group of balance laws.

4.1. Momentum Balance Laws

The source term $\hat{m}_{bi}$ computed in (47) from an extended thermodynamics point of view can be rewritten

$$\begin{aligned} \hat{m}^{\text{lin}}_{bi} &= - \sum_{c=1}^{n-1} \psi_{bc}(\mathbf{w}_{\text{E}}) \frac{u_{ci} - u_{ni}}{T} \\ &= \sum_{\substack{c=1 \\ c\neq b}}^{n-1} \left(-\frac{\psi_{bc}(\mathbf{w}_{\text{E}})}{T} \right) (u_{ci} - u_{bi}) + \left(\sum_{c=1}^{n-1} \frac{\psi_{bc}(\mathbf{w}_{\text{E}})}{T} \right) (u_{ni} - u_{bi}). \end{aligned}$$

Transforming (82) in a similar way, taking into account $v_\alpha - v_\beta = \mathbf{u}_\alpha - \mathbf{u}_\beta$, one obtains

$$\begin{aligned}\mathfrak{m}^{\text{lin}}_{\alpha} &= -\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n} \rho_\alpha \rho_\beta\, \mathcal{M}_{\alpha\beta}\, T^{\frac{\gamma_{\alpha\beta}}{2}}\, (v_\alpha - v_\beta) \\ &= -\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n-1} \rho_\alpha \rho_\beta\, \mathcal{M}_{\alpha\beta}\, T^{\frac{\gamma_{\alpha\beta}}{2}}\, (\mathbf{u}_\alpha - \mathbf{u}_\beta) - \rho_\alpha \rho_n\, \mathcal{M}_{\alpha n}\, T^{\frac{\gamma_{\alpha n}}{2}}\, (\mathbf{u}_\alpha - \mathbf{u}_n)\end{aligned} \tag{85}$$

Using the equality $\hat{\mathfrak{m}}^{\text{lin}}_{bi} = \mathfrak{m}^{\text{lin}}_{\alpha}$, after straightforward computation the following form of phenomenological coefficients is obtained

$$\psi_{bc}(\mathbf{w}_{\text{E}}) = \begin{cases} -\rho_b \rho_c\, \mathcal{M}_{bc}\, T^{\frac{\gamma_{bc}}{2}+1}, & c \neq b, \\ \sum\limits_{\substack{d=1\\ d\neq b}}^{n} \rho_b \rho_d \mathcal{M}_{bd} T^{\frac{\gamma_{bd}}{2}+1}, & c = b, \end{cases} \tag{86}$$

for $b, c \in \{1, \ldots, n-1\}$, where the constant $\mathcal{M}_{bc} > 0$ is from (A23). It is symmetric with respect to (b, c), which implies that matrix $[\psi_{bc}]_{1 \leq b,c \leq n-1}$ is symmetric as well.

4.2. Energy Balance Laws

First, we rewrite the linearized form of energy production term (48) of extended thermodynamics, by exploiting the relation (65) between specific internal energy density and pressure, i.e.,

$$\frac{k_{\text{B}}}{m_c}\frac{\rho_c}{p_{c\text{E}}^2} = \frac{m_c}{k_{\text{B}}}\frac{1}{\rho_c T^2}, \quad \frac{k_{\text{B}}}{m_c}\frac{1}{p_{c\text{E}}\varepsilon_{c\text{E}}} = \frac{2}{2a_c+5}\frac{m_c}{k_{\text{B}}}\frac{1}{\rho_c T^2}$$

implying

$$\begin{aligned}\hat{e}^{\text{lin}}_{b} = &\sum_{c=1}^{n-1} \frac{\theta^{e}_{bc}(\mathbf{w}_{\text{E}})}{T^2}\left\{-\Theta_c + \Theta_n + \tilde{A}_c \frac{m_c}{k_{\text{B}}}\frac{\Pi_c}{\rho_c} - \tilde{A}_n \frac{m_n}{k_{\text{B}}}\frac{\Pi_n}{\rho_n}\right\} \\ &- \sum_{c=1}^{n-1} \frac{\theta^{M}_{bc}(\mathbf{w}_{\text{E}})}{T^2}\left\{A_c \frac{m_c}{k_{\text{B}}}\frac{\Pi_c}{\rho_c} - A_n \frac{m_n}{k_{\text{B}}}\frac{\Pi_n}{\rho_n}\right\},\end{aligned}$$

with notation

$$A_c = \frac{2a_c+5}{4(a_c+1)}, \quad \tilde{A}_c = \frac{3}{2(a_c+1)}. \tag{87}$$

Adding and subtracting suitable terms, $\hat{e}^{\text{lin}}_{b}$ can be transformed to

$$\begin{aligned}\hat{e}^{\text{lin}}_{b} = &\sum_{\substack{c=1\\ c\neq b}}^{n-1} \frac{\theta^{e}_{bc}(\mathbf{w}_{\text{E}})}{T^2}\left\{\Theta_b - \tilde{A}_b \frac{m_b}{k_{\text{B}}}\frac{\Pi_b}{\rho_b} - \left(\Theta_c - \tilde{A}_c \frac{m_c}{k_{\text{B}}}\frac{\Pi_c}{\rho_c}\right)\right\} \\ &+ \sum_{\substack{c=1\\ c\neq b}}^{n-1} \frac{\theta^{M}_{bc}(\mathbf{w}_{\text{E}})}{T^2}\left\{A_b \frac{m_b}{k_{\text{B}}}\frac{\Pi_b}{\rho_b} - A_c \frac{m_c}{k_{\text{B}}}\frac{\Pi_c}{\rho_c}\right\} \\ &- \left(\sum_{c=1}^{n-1} \frac{\theta^{e}_{bc}(\mathbf{w}_{\text{E}})}{T^2}\right)\left\{\Theta_b - \tilde{A}_b \frac{m_b}{k_{\text{B}}}\frac{\Pi_b}{\rho_b} - \left(\Theta_n - \tilde{A}_n \frac{m_n}{k_{\text{B}}}\frac{\Pi_n}{\rho_n}\right)\right\} \\ &- \left(\sum_{c=1}^{n-1} \frac{\theta^{M}_{bc}(\mathbf{w}_{\text{E}})}{T^2}\right)\left\{A_b \frac{m_b}{k_{\text{B}}}\frac{\Pi_b}{\rho_b} - A_n \frac{m_n}{k_{\text{B}}}\frac{\Pi_n}{\rho_n}\right\}.\end{aligned} \tag{88}$$

On the other side, the linearized energy production term (84), computed by evaluating the Boltzmann collision operator, can be presented as $\mathfrak{e}_\alpha^{\mathrm{lin}} = \boldsymbol{v} \cdot \mathfrak{m}_\alpha^{\mathrm{lin}} + \hat{\mathfrak{e}}_\alpha^{\mathrm{lin}}$ and the velocity independent part can be written as

$$\begin{aligned}
\hat{\mathfrak{e}}_\alpha^{\mathrm{lin}} = &-\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n-1} \rho_\alpha \rho_\beta \, T^{\frac{\gamma_{\alpha\beta}}{2}} \, \mathcal{E}_{\alpha\beta}^{T} \left\{ \Theta_\alpha - \tilde{A}_\alpha \frac{m_\alpha}{k_B} \frac{\Pi_\alpha}{\rho_\alpha} - \left(\Theta_\beta - \tilde{A}_\beta \frac{m_\beta}{k_B} \frac{\Pi_\beta}{\rho_\beta} \right) \right\} \\
&-\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n-1} \rho_\alpha \rho_\beta \, T^{\frac{\gamma_{\alpha\beta}}{2}} \left\{ \left(\tilde{A}_\alpha \mathcal{E}_{\alpha\beta}^{T} - \mathcal{E}_{\alpha\beta}^{\Pi} \right) \frac{m_\alpha}{k_B} \frac{\Pi_\alpha}{\rho_\alpha} - \left(\tilde{A}_\beta \mathcal{E}_{\alpha\beta}^{T} - \mathcal{E}_{\beta\alpha}^{\Pi} \right) \frac{m_\beta}{k_B} \frac{\Pi_\beta}{\rho_\beta} \right\} \\
&- \rho_\alpha \rho_n \, T^{\frac{\gamma_{\alpha n}}{2}} \, \mathcal{E}_{\alpha n}^{T} \left\{ \Theta_\alpha - \tilde{A}_\alpha \frac{m_\alpha}{k_B} \frac{\Pi_\alpha}{\rho_\alpha} - \left(\Theta_n - \tilde{A}_n \frac{m_n}{k_B} \frac{\Pi_n}{\rho_n} \right) \right\} \\
&- \rho_\alpha \rho_n \, T^{\frac{\gamma_{\alpha n}}{2}} \left\{ \left(\tilde{A}_\alpha \mathcal{E}_{\alpha n}^{T} - \mathcal{E}_{\alpha n}^{\Pi} \right) \frac{m_\alpha}{k_B} \frac{\Pi_\alpha}{\rho_\alpha} - \left(\tilde{A}_n \mathcal{E}_{\alpha n}^{T} - \mathcal{E}_{n\alpha}^{\Pi} \right) \frac{m_n}{k_B} \frac{\Pi_n}{\rho_n} \right\}.
\end{aligned} \tag{89}$$

From (88) and (89), equality $\hat{e}_b^{\mathrm{lin}} = \hat{\mathfrak{e}}_b^{\mathrm{lin}}$ yields explicit form of phenomenological coefficients. Firstly the expression for off-diagonal terms of θ_{bc}^{e},

$$\theta_{bc}^{e}(\mathbf{w}_{\mathrm{E}}) = -\rho_b \rho_c \, \mathcal{E}_{bc}^{T} \, T^{\frac{\gamma_{bc}}{2}+2}, \quad \text{for } b, c \in \{1, \dots, n-1\} \text{ and } b \neq c. \tag{90}$$

Off-diagonal terms of θ_{bc}^{M} are obtained from the system

$$\begin{aligned}
\rho_b \rho_c T^{\frac{\gamma_{bc}}{2}} \left(\tilde{A}_b \mathcal{E}_{bc}^{T} - \mathcal{E}_{bc}^{\Pi} \right) &= -\frac{\theta_{bc}^{M}(\mathbf{w}_{\mathrm{E}})}{T^2} A_b, \\
\rho_b \rho_c T^{\frac{\gamma_{bc}}{2}} \left(\tilde{A}_c \mathcal{E}_{bc}^{T} - \mathcal{E}_{cb}^{\Pi} \right) &= -\frac{\theta_{bc}^{M}(\mathbf{w}_{\mathrm{E}})}{T^2} A_c,
\end{aligned}$$

Since these two equations have to be compatible, one obtains

$$\frac{\theta_{bc}^{M}(\mathbf{w}_{\mathrm{E}})}{T^2} = \rho_b \rho_c T^{\frac{\gamma_{bc}}{2}} \frac{\mathcal{E}_{bc}^{\Pi} \tilde{A}_c - \mathcal{E}_{cb}^{\Pi} \tilde{A}_b}{A_b \tilde{A}_c - A_c \tilde{A}_b},$$

or explicitly

$$\theta_{bc}^{M}(\mathbf{w}_{\mathrm{E}}) = \rho_b \rho_c T^{\frac{\gamma_{bc}}{2}+2} \, \frac{2(a_b+1)\mathcal{E}_{bc}^{\Pi} - 2(a_c+1)\mathcal{E}_{cb}^{\Pi}}{a_b - a_c}, \tag{91}$$

for $b, c \in \{1, \dots, n-1\}$ and $b \neq c$. Exploiting further comparison of (88) and (89), diagonal terms are obtained, for any $b \in \{1, \dots, n-1\}$,

$$\theta_{bb}^{e}(\mathbf{w}_{\mathrm{E}}) = \rho_b \rho_n \, \mathcal{E}_{bn}^{T} \, T^{\frac{\gamma_{bn}}{2}+2} - \sum_{\substack{d=1\\ d\neq b}}^{n-1} \theta_{bd}^{e}(\mathbf{w}_{\mathrm{E}}),$$

or explicitly

$$\theta_{bb}^{e}(\mathbf{w}_{\mathrm{E}}) = \rho_b \sum_{\substack{d=1\\ d\neq b}}^{n} \rho_d \, \mathcal{E}_{bd}^{T} \, T^{\frac{\gamma_{bd}}{2}+2}, \tag{92}$$

and similarly

$$\theta_{bb}^{M}(\mathbf{w}_{\mathrm{E}}) = -\rho_b \sum_{\substack{d=1\\ d\neq b}}^{n} \rho_d \, T^{\frac{\gamma_{bd}}{2}+2} \, \frac{2(a_b+1)\mathcal{E}_{bd}^{\Pi} - 2(a_d+1)\mathcal{E}_{db}^{\Pi}}{a_b - a_d}. \tag{93}$$

4.3. Dynamic Pressure Balance Laws

In the same fashion as in the case of energy balance laws, the source term $\hat{M}_b^{\mathrm{lin}}$ from (46) can be transformed into

$$\begin{aligned}\hat{M}_b^{\mathrm{lin}} = &\sum_{c=1}^{n-1} \frac{\chi_{bc}^{e}(\mathbf{w}_{\mathrm{E}})}{T^2}\left\{-\Theta_c + \Theta_n + \tilde{A}_c \frac{m_c}{k_{\mathrm{B}}}\frac{\Pi_c}{\rho_c} - \tilde{A}_n \frac{m_n}{k_{\mathrm{B}}}\frac{\Pi_n}{\rho_n}\right\} \\ &- \sum_{c=1}^{n-1} \frac{\chi_{bc}^{M}(\mathbf{w}_{\mathrm{E}})}{T^2}\left\{A_c \frac{m_c}{k_{\mathrm{B}}}\frac{\Pi_c}{\rho_c} - A_n \frac{m_n}{k_{\mathrm{B}}}\frac{\Pi_n}{\rho_n}\right\},\end{aligned} \tag{94}$$

with notation (87), while (46) becomes

$$\hat{P}_\alpha^{\mathrm{lin}} = -\frac{\omega_\alpha(\mathbf{w}_{\alpha\mathrm{E}})}{T^2} A_\alpha \frac{m_\alpha}{k_{\mathrm{B}}}\frac{\Pi_\alpha}{\rho_\alpha}. \tag{95}$$

Therefore, we may write

$$\begin{aligned}\hat{P}_b^{\mathrm{lin}} + \hat{M}_b^{\mathrm{lin}} = &\sum_{\substack{c=1\\c\neq b}}^{n-1} \frac{\chi_{bc}^{e}(\mathbf{w}_{\mathrm{E}})}{T^2}\left\{\Theta_b - \tilde{A}_b \frac{m_b}{k_{\mathrm{B}}}\frac{\Pi_b}{\rho_b} - \left(\Theta_c - \tilde{A}_c \frac{m_c}{k_{\mathrm{B}}}\frac{\Pi_c}{\rho_c}\right)\right\} \\ &+ \sum_{\substack{c=1\\c\neq b}}^{n-1} \frac{\chi_{bc}^{M}(\mathbf{w}_{\mathrm{E}})}{T^2}\left\{A_b \frac{m_b}{k_{\mathrm{B}}}\frac{\Pi_b}{\rho_b} - A_c \frac{m_c}{k_{\mathrm{B}}}\frac{\Pi_c}{\rho_c}\right\} \\ &- \left(\sum_{c=1}^{n-1} \frac{\chi_{bc}^{e}(\mathbf{w}_{\mathrm{E}})}{T^2}\right)\left\{\Theta_b - \tilde{A}_b \frac{m_b}{k_{\mathrm{B}}}\frac{\Pi_b}{\rho_b} - \left(\Theta_n - \tilde{A}_n \frac{m_n}{k_{\mathrm{B}}}\frac{\Pi_n}{\rho_n}\right)\right\} \\ &- \left(\sum_{c=1}^{n-1} \frac{\chi_{bc}^{M}(\mathbf{w}_{\mathrm{E}})}{T^2}\right)\left\{A_b \frac{m_b}{k_{\mathrm{B}}}\frac{\Pi_b}{\rho_b} - A_n \frac{m_n}{k_{\mathrm{B}}}\frac{\Pi_n}{\rho_n}\right\} - \frac{\omega_b(\mathbf{w}_{b\mathrm{E}})}{T^2} A_b \frac{m_b}{k_{\mathrm{B}}}\frac{\Pi_b}{\rho_b}.\end{aligned} \tag{96}$$

On the other side, (83) can be recast as $\mathfrak{P}_\alpha^{\mathrm{lin}} = 2\boldsymbol{v} \cdot \mathfrak{m}_\alpha^{\mathrm{lin}} + \hat{\mathfrak{P}}_\alpha^{\mathrm{lin}}$ where $\hat{\mathfrak{P}}_\alpha^{\mathrm{lin}}$ reads

$$\begin{aligned}\hat{\mathfrak{P}}_\alpha^{\mathrm{lin}} = &-\sum_{\substack{\beta=1\\\beta\neq\alpha}}^{n-1} \rho_\alpha\rho_\beta\, T^{\frac{\gamma_{\alpha\beta}}{2}} \mathcal{P}_{\alpha\beta}^{T}\left\{\Theta_\alpha - \tilde{A}_\alpha \frac{m_\alpha}{k_{\mathrm{B}}}\frac{\Pi_\alpha}{\rho_\alpha} - \left(\Theta_\beta - \tilde{A}_\beta \frac{m_\beta}{k_{\mathrm{B}}}\frac{\Pi_\beta}{\rho_\beta}\right)\right\} \\ &- \sum_{\substack{\beta=1\\\beta\neq\alpha}}^{n-1} \rho_\alpha\rho_\beta\, T^{\frac{\gamma_{\alpha\beta}}{2}}\left\{\left(\tilde{A}_\alpha \mathcal{P}_{\alpha\beta}^{T} + \mathcal{P}_{\alpha\beta}^{\Pi}\right)\frac{m_\alpha}{k_{\mathrm{B}}}\frac{\Pi_\alpha}{\rho_\alpha} - \left(\tilde{A}_\beta \mathcal{P}_{\alpha\beta}^{T} + \tilde{\mathcal{P}}_{\alpha\beta}^{\Pi}\right)\frac{m_\beta}{k_{\mathrm{B}}}\frac{\Pi_\beta}{\rho_\beta}\right\} \\ &- \rho_\alpha\rho_n\, T^{\frac{\gamma_{\alpha n}}{2}} \mathcal{P}_{\alpha n}^{T}\left\{\Theta_\alpha - \tilde{A}_\alpha \frac{m_\alpha}{k_{\mathrm{B}}}\frac{\Pi_\alpha}{\rho_\alpha} - \left(\Theta_n - \tilde{A}_n \frac{m_n}{k_{\mathrm{B}}}\frac{\Pi_n}{\rho_n}\right)\right\} \\ &- \rho_\alpha\rho_n\, T^{\frac{\gamma_{\alpha n}}{2}}\left\{\left(\tilde{A}_\alpha \mathcal{P}_{\alpha n}^{T} + \mathcal{P}_{\alpha n}^{\Pi}\right)\frac{m_\alpha}{k_{\mathrm{B}}}\frac{\Pi_\alpha}{\rho_\alpha} - \left(\tilde{A}_n \mathcal{P}_{\alpha n}^{T} + \tilde{\mathcal{P}}_{\alpha n}^{\Pi}\right)\frac{m_n}{k_{\mathrm{B}}}\frac{\Pi_n}{\rho_n}\right\}.\end{aligned} \tag{97}$$

From (96) and (97), and equality $\hat{P}_b^{\mathrm{lin}} + \hat{M}_b^{\mathrm{lin}} = \hat{\mathfrak{P}}_b^{\mathrm{lin}}$ we may compute the phenomenological coefficients. A straightforward application of the same procedure as in energy balance laws yields the following form of the coefficients $\chi_{bc}^{e}(\mathbf{w}_{\mathrm{E}})$

$$\chi_{bc}^{e}(\mathbf{w}_{\mathrm{E}}) = \begin{cases} -\rho_b\rho_c\, \mathcal{P}_{bc}^{T}\, T^{\frac{\gamma_{bc}}{2}+2}, & c \neq b, \\ \displaystyle\sum_{\substack{d=1\\d\neq b}}^{n} \rho_b\rho_d\, \mathcal{P}_{bd}^{T}\, T^{\frac{\gamma_{bd}}{2}+2}, & c = b, \end{cases} \tag{98}$$

for $b, c \in \{1, \ldots, n-1\}$. For computation the off-diagonal terms $\chi^M_{bc}(\mathbf{w}_{\mathrm{E}})$ we obtain two equations:

$$
\begin{aligned}
-\rho_b\rho_c T^{\frac{\gamma_{bc}}{2}}\left(\tilde{A}_b\mathcal{P}^T_{bc} + \mathcal{P}^{\Pi}_{bc}\right) &= \frac{\chi^M_{bc}(\mathbf{w}_{\mathrm{E}})}{T^2}A_b, \\
-\rho_b\rho_c T^{\frac{\gamma_{bc}}{2}}\left(\tilde{A}_c\mathcal{P}^T_{bc} + \tilde{\mathcal{P}}^{\Pi}_{bc}\right) &= \frac{\chi^M_{bc}(\mathbf{w}_{\mathrm{E}})}{T^2}A_c.
\end{aligned}
$$

As a consequence of their compatibility, we obtain

$$
\begin{aligned}
\chi^M_{bc}(\mathbf{w}_{\mathrm{E}}) &= -\rho_b\rho_c T^{\frac{\gamma_{bc}}{2}+2}\frac{\mathcal{P}^{\Pi}_{bc}\tilde{A}_c - \tilde{\mathcal{P}}^{\Pi}_{bc}\tilde{A}_b}{A_b\tilde{A}_c - A_c\tilde{A}_b} \\
&= -2\rho_b\rho_c T^{\frac{\gamma_{bc}}{2}+2}\left(\mathcal{P}^T_{bc} + \frac{2\,m_c(1+a_b)(1+a_c)}{3(a_b-a_c)}\mathcal{P}^{\chi}_{bc}\right),
\end{aligned}
\tag{99}
$$

where the last expression is obtained thanks to computation performed in (A26) with $\mathcal{P}^{\chi}_{bc} > 0$ symmetric in (b, c) and given in (A27).

Further comparison leads us to the following system of equations

$$
\begin{aligned}
\rho_b\rho_n T^{\frac{\gamma_{bn}}{2}}\left(\tilde{A}_b\mathcal{P}^T_{bn} + \mathcal{P}^{\Pi}_{bn}\right) &= \left\{\left(\sum_{c=1}^{n-1}\frac{\chi^e_{bc}(\mathbf{w}_{\mathrm{E}})}{T^2}\right) + \frac{\omega_b(\mathbf{w}_{b\mathrm{E}})}{T^2}\right\}A_b, \\
\rho_b\rho_n T^{\frac{\gamma_{bn}}{2}}\left(\tilde{A}_n\mathcal{P}^T_{bn} + \tilde{\mathcal{P}}^{\Pi}_{bn}\right) &= \left(\sum_{c=1}^{n-1}\frac{\chi^e_{bc}(\mathbf{w}_{\mathrm{E}})}{T^2}\right)A_n.
\end{aligned}
$$

By first eliminating $\chi^M_{bc}(\mathbf{w}_{\mathrm{E}})$ one obtains

$$
\begin{aligned}
\omega_b(\mathbf{w}_{b\mathrm{E}}) &= \frac{\rho_b\rho_n}{A_bA_n}T^{\frac{\gamma_{bc}}{2}+2}\left[(\tilde{A}_bA_n - \tilde{A}_nA_b)\mathcal{P}^T_{bn} + \mathcal{P}^{\Pi}_{bn}A_n - \tilde{\mathcal{P}}^{\Pi}_{bn}A_b\right] \\
&= \rho_b\rho_n T^{\frac{\gamma_{bn}}{2}+2}m_n\mathcal{P}^{\omega}_{bn},
\end{aligned}
\tag{100}
$$

after involving (A28) with $\mathcal{P}^{\omega}_{bn} > 0$ given in (A29). Note that coefficients $\omega_b(\mathbf{w}_{b\mathrm{E}})$ given in (100) formally depend on constituent-related objective quantities in equilibrium, since the properties of component n do not enter into the description of the mixture and can be treated as parameters.

With this result at hand, compatibility of the equations leads to diagonal phenomenological coefficients

$$
\begin{aligned}
\chi^M_{bb}(\mathbf{w}_{\mathrm{E}}) &= \sum_{\substack{d=1\\ d\neq b}}^{n}\rho_b\rho_d T^{\frac{\gamma_{bd}}{2}+2}\frac{\mathcal{P}^{\Pi}_{bd}\tilde{A}_d - \tilde{\mathcal{P}}^{\Pi}_{bd}\tilde{A}_b}{A_b\tilde{A}_d - A_d\tilde{A}_b} - \omega_b(\mathbf{w}_{b\mathrm{E}})\frac{A_b\tilde{A}_n}{A_b\tilde{A}_n - A_n\tilde{A}_b} \\
&= -2\sum_{\substack{d=1\\ d\neq b}}^{n}\rho_b\rho_d T^{\frac{\gamma_{bd}}{2}+2}\left(\mathcal{P}^T_{bd} + \frac{2\,m_d(1+a_b)(1+a_d)}{3(a_b-a_d)}\mathcal{P}^{\chi}_{bd}\right) \\
&\quad - \frac{a_b+\frac{5}{2}}{a_b-a_n}\rho_b\rho_n T^{\frac{\gamma_{bn}}{2}+2}m_n\mathcal{P}^{\omega}_{bn},
\end{aligned}
\tag{101}
$$

with constants defined in (A25), (A27), and (A29).

5. Conclusions

In this paper, we studied the mixture of polyatomic gases with dynamic pressure. It was assumed that a macroscopic set of field variables consists of mass densities, velocities, temperatures, and dynamic pressures of the constituents. This enabled a complete comparison of two different approaches to mixture modeling—a macroscopic approach within the framework of extended thermodynamics, and a mesoscopic approach based on the kinetic theory of mixtures of polyatomic gases. First, the model was developed using the methods of extended thermodynamics and closed using the entropy principle. Second, the kinetic model is established starting from the maximum entropy principle, which facilitated the construction of approximate distribution functions compatible with macroscopic field variables. After that, equivalent macroscopic equations were derived as moment equations of the system of Boltzmann equations. Finally, a novel macroscopic/kinetic method, recently established by the authors, was applied to achieve complete closure of the macroscopic equations derived in extended thermodynamics.

The results of this study are new in several aspects. In the context of rational thermodynamics, Truesdell's metaphysical principles are for the first time extended to dissipative systems of hyperbolic (relaxation) type. In the context of kinetic theory, the model of polyatomic gases with a single scalar variable describing internal molecular energy was systematically applied to mixtures and yielded the exact closure in the desired approximation. Promising recent results in transport coefficient modeling based on the evaluation of the single polyatomic Boltzmann collision operator are extended in this paper to the case of a polyatomic gas mixture. Finally, the combination of these two approaches leads to a procedure for the complete closure of macroscopic equations derived in the framework of extended thermodynamics. This is an important result since one cannot rely on other approaches (e.g. experimental evidence) to obtain an explicit form of the phenomenological coefficients.

It has to be noted that the computation of the phenomenological coefficients in this study is of a formal kind. There remains to prove the positive semi-definiteness of the coefficient matrices, which is a subject of ongoing study. Furthermore, the closed form of governing equations now provides the possibility for numerical simulation of different processes in mixtures, which take into account cross-diffusion, multi-temperature effects, and internal dissipation described through the presence of dynamic pressure and bulk viscosity.

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Appendix A. Main Feld

From the structure of main field (33) and relations (40), the following form of the main field of the system (18) and (19) is obtained:

$$\begin{aligned}
\lambda &= -\frac{1}{T_n}\left(g_n - \frac{1}{2}|\mathbf{v}+\mathbf{u}_n|^2\right) - \left(\varepsilon_n - \frac{1}{2}|\mathbf{v}+\mathbf{u}_n|^2\right)\left(\frac{\partial k_n}{\partial \varepsilon_n} - \frac{\partial k_n}{\partial \Pi_n}\frac{\partial p_n}{\partial \varepsilon_n}\right)\\
&\quad - \rho_n \frac{\partial k_n}{\partial \Pi_n}\left(\frac{\partial p_n}{\partial \rho_n} - \frac{1}{3}|\mathbf{v}+\mathbf{u}_n|^2\right) + k_n + \rho_n \frac{\partial k_n}{\partial \rho_n},\\
\Lambda_i &= -\frac{v_i + u_{ni}}{T_n} - \left(\frac{\partial k_n}{\partial \varepsilon_n} - \frac{\partial k_n}{\partial \Pi_n}\frac{\partial p_n}{\partial \varepsilon_n} + \frac{2}{3}\rho_n \frac{\partial k_n}{\partial \Pi_n}\right)(v_i + u_{ni}),\\
\mu &= \frac{1}{T_n} + \frac{\partial k_n}{\partial \varepsilon_n} - \frac{\partial k_n}{\partial \Pi_n}\frac{\partial p_n}{\partial \varepsilon_n},\\
\zeta &= \frac{1}{3}\rho_n \frac{\partial k_n}{\partial \Pi_n},
\end{aligned} \tag{A1}$$

and

$$\begin{aligned}
\lambda_b &= -\frac{1}{T_b}\left(g_b - \frac{1}{2}|\mathbf{v}+\mathbf{u}_b|^2\right) - \left(\varepsilon_b - \frac{1}{2}|\mathbf{v}+\mathbf{u}_b|^2\right)\left(\frac{\partial k_b}{\partial \varepsilon_b} - \frac{\partial k_b}{\partial \Pi_b}\frac{\partial p_b}{\partial \varepsilon_b}\right)\\
&\quad - \rho_b \frac{\partial k_b}{\partial \Pi_b}\left(\frac{\partial p_b}{\partial \rho_b} - \frac{1}{3}|\mathbf{v}+\mathbf{u}_b|^2\right) + k_b + \rho_b \frac{\partial k_b}{\partial \rho_b}\\
&\quad + \frac{1}{T_n}\left(g_n - \frac{1}{2}|\mathbf{v}+\mathbf{u}_n|^2\right) + \left(\varepsilon_n - \frac{1}{2}|\mathbf{v}+\mathbf{u}_n|^2\right)\left(\frac{\partial k_n}{\partial \varepsilon_n} - \frac{\partial k_n}{\partial \Pi_n}\frac{\partial p_n}{\partial \varepsilon_n}\right)\\
&\quad + \rho_n \frac{\partial k_n}{\partial \Pi_n}\left(\frac{\partial p_n}{\partial \rho_n} - \frac{1}{3}|\mathbf{v}+\mathbf{u}_n|^2\right) - k_n - \rho_n \frac{\partial k_n}{\partial \rho_n},\\
\Lambda_{bi} &= -\frac{v_i + u_{bi}}{T_b} - \left(\frac{\partial k_b}{\partial \varepsilon_b} - \frac{\partial k_b}{\partial \Pi_b}\frac{\partial p_b}{\partial \varepsilon_b} + \frac{2}{3}\rho_b \frac{\partial k_b}{\partial \Pi_b}\right)(v_i + u_{bi})\\
&\quad + \frac{v_i + u_{ni}}{T_n} + \left(\frac{\partial k_n}{\partial \varepsilon_n} - \frac{\partial k_n}{\partial \Pi_n}\frac{\partial p_n}{\partial \varepsilon_n} + \frac{2}{3}\rho_n \frac{\partial k_n}{\partial \Pi_n}\right)(v_i + u_{ni}),\\
\mu_b &= \frac{1}{T_b} + \frac{\partial k_b}{\partial \varepsilon_b} - \frac{\partial k_b}{\partial \Pi_b}\frac{\partial p_b}{\partial \varepsilon_b} - \frac{1}{T_n} - \frac{\partial k_n}{\partial \varepsilon_n} + \frac{\partial k_n}{\partial \Pi_n}\frac{\partial p_n}{\partial \varepsilon_n},\\
\zeta_b &= \frac{1}{3}\rho_b \frac{\partial k_b}{\partial \Pi_b} - \frac{1}{3}\rho_n \frac{\partial k_n}{\partial \Pi_n}.
\end{aligned} \tag{A2}$$

In the derivation of linearized source terms for a non-reacting mixture, we need the components of the main field linearized in the neighborhood of equilibrium state $\mathbf{u}_{\mathrm{E}} = (\rho, \mathbf{v}, \varepsilon, 0, \rho_b, \mathbf{0}, T, 0)$. Taking into account (A2) and (36), we obtain:

$$\begin{aligned}
\hat{\Lambda}_{bi} &\approx -\frac{u_{bi} - u_{ni}}{T},\\
\hat{\mu}_b &\approx -\frac{\Theta_b - \Theta_n}{T^2}\\
&\quad + \frac{3}{2}\frac{k_{\mathrm{B}}}{m_b}\left(1 + \frac{3}{2(a_b+1)}\right)\frac{\Pi_b}{p_{b\mathrm{E}}\varepsilon_{b\mathrm{E}}} - \frac{3}{2}\frac{k_{\mathrm{B}}}{m_n}\left(1 + \frac{3}{2(a_n+1)}\right)\frac{\Pi_n}{p_{n\mathrm{E}}\varepsilon_{n\mathrm{E}}},\\
\hat{\zeta}_b &\approx -\frac{1}{2}\frac{k_{\mathrm{B}}}{m_b}\left(1 + \frac{3}{2(a_b+1)}\right)\frac{\rho_b}{p_{b\mathrm{E}}^2}\Pi_b + \frac{1}{2}\frac{k_{\mathrm{B}}}{m_n}\left(1 + \frac{3}{2(a_n+1)}\right)\frac{\rho_n}{p_{n\mathrm{E}}^2}\Pi_n,
\end{aligned} \tag{A3}$$

where $u_{\alpha i} = v_{\alpha i} - v_i$ and $\Theta_\alpha = T_\alpha - T$.

Appendix B. Hypergeometric Functions

Following [45], p. 505, relation 13.2.1, we define the Kummer confluent hypergeometric function, denoted by ${}_1F_1(a,b,z)$, with its integral representation

$$\frac{\Gamma(b-a)\Gamma(a)}{\Gamma(b)}\,{}_1F_1(a,b,z) = \int_0^1 e^{zt}t^{a-1}(1-t)^{b-a-1}\mathrm{d}t, \tag{A4}$$

for $b > a > 0$. Next, we introduce the following function

$${}_0\tilde{F}_1(b,z) = \frac{1}{\Gamma[b]}e^{-2\sqrt{z}}\,{}_1F_1\Big(b-\tfrac{1}{2}, 2b-1, 4\sqrt{z}\Big). \tag{A5}$$

The two hypergeometric functions are connected through the integral representation

$${}_1\tilde{F}_1(a,b,z) = \frac{1}{\Gamma[a]}\int_0^\infty e^{-t}\,t^{a-1}\,{}_0\tilde{F}_1(b,zt)\mathrm{d}t, \tag{A6}$$

for $a > 0$.

Appendix C. Calculation of the Production Terms

For the sake of simplicity, we introduce the following positive constants

$$\begin{aligned} U_\alpha &= \frac{m_\alpha}{2k_BT_\alpha}\left(1+\frac{\Pi_\alpha}{p_\alpha}\right)^{-1}, \qquad V_\alpha = \frac{1}{k_BT_\alpha}\left(1-\frac{3}{2}\frac{\Pi_\alpha}{(a_\alpha+1)p_\alpha}\right)^{-1}, \\ W_\alpha &= \frac{\rho_\alpha}{m_\alpha}\frac{U_\alpha^{3/2}}{\pi^{3/2}}\frac{V_\alpha^{a_\alpha+1}}{\Gamma(a_\alpha+1)}, \end{aligned} \tag{A7}$$

that allows to rewrite (70) as

$$\hat{f}_\alpha^6 = W_\alpha I^{a_\alpha} e^{-U_\alpha|\boldsymbol{\xi}-\boldsymbol{v}_\alpha|^2 - V_\alpha I}.$$

The aim of this section is to calculate the production terms (67) for the choice of this distribution function and the collision kernel (73), namely to compute

$$\begin{pmatrix} \mathfrak{m}_\alpha \\ \mathfrak{P}_\alpha \\ \tilde{\mathfrak{e}}_\alpha \end{pmatrix} = \sum_\beta W_\alpha W_\beta \int_{\Delta^2\times K}\begin{pmatrix} m_\alpha(\boldsymbol{\xi}'-\boldsymbol{\xi}) \\ m_\alpha\left(|\boldsymbol{\xi}'|^2-|\boldsymbol{\xi}|^2\right) \\ I'-I \end{pmatrix}$$
$$\times\, e^{-U_\alpha|\boldsymbol{\xi}-\boldsymbol{v}_\alpha|^2 - U_\beta|\boldsymbol{\xi}_*-\boldsymbol{v}_\beta|^2} I^{a_\alpha} I_*^{a_\beta} e^{-V_\alpha I - V_\beta I_*}\mathcal{B}_{\alpha\beta}\,\psi_{\alpha\beta}\mathrm{d}R\,\mathrm{d}r\,\mathrm{d}\sigma\,\mathrm{d}I_*\,\mathrm{d}\boldsymbol{\xi}_*\,\mathrm{d}I\,\mathrm{d}\boldsymbol{\xi},$$

We will work in the center-of-mass reference frame. To that end, we introduce variables **g** and **G** as in (53). We first rewrite the exponent of exponentials,

$$U_\alpha|\boldsymbol{\xi}-\boldsymbol{v}_\alpha|^2 + U_\beta|\boldsymbol{\xi}_*-\boldsymbol{v}_\beta|^2 = a_{\alpha\beta}|\mathbf{g}+\mathbf{b}_{\alpha\beta}|^2 + c_{\alpha\beta}|\mathbf{G}+d_{\alpha\beta}\mathbf{g}+\mathbf{e}_{\alpha\beta}|^2,$$

for the following choice of the coefficients

$$\begin{aligned} a_{\alpha\beta} &= \left(\frac{1}{U_\alpha}+\frac{1}{U_\beta}\right)^{-1}, \quad \mathbf{b}_{\alpha\beta} = \boldsymbol{v}_\beta - \boldsymbol{v}_\alpha, \quad c_{\alpha\beta} = U_\alpha + U_\beta, \\ d_{\alpha\beta} &= \mu_{\alpha\beta}(U_\alpha+U_\beta)^{-1}\left(\frac{U_\alpha}{m_\alpha}-\frac{U_\beta}{m_\beta}\right), \quad \mathbf{e}_{\alpha\beta} = -(U_\alpha+U_\beta)^{-1}(U_\alpha\boldsymbol{v}_\alpha + U_\beta\boldsymbol{v}_\beta). \end{aligned} \tag{A8}$$

Using the collisional rules (52), the test functions become

$$\begin{aligned} m_\alpha(\boldsymbol{\xi}' - \boldsymbol{\xi}) &= \mu_{\alpha\beta}\left(-\mathbf{g} + \sqrt{\frac{2RE}{\mu_{\alpha\beta}}}\sigma\right), \\ m_\alpha\left(\left|\boldsymbol{\xi}'\right|^2 - |\boldsymbol{\xi}|^2\right) &= 2\sqrt{2\mu_{\alpha\beta}RE}\,\mathbf{G}\cdot\sigma - 2\mu_{\alpha\beta}\mathbf{G}\cdot\mathbf{g} \\ &\qquad + 2\frac{m_\beta}{m_\alpha + m_\beta}R(I + I_*) - \mu_{\alpha\beta}\frac{m_\beta}{m_\alpha + m_\beta}(1 - R)|\mathbf{g}|^2, \\ I' - I &= \frac{\mu_{\alpha\beta}}{2}r(1 - R)|\mathbf{g}|^2 - (1 - r(1 - R))I + r(1 - R)I_*. \end{aligned} \tag{A9}$$

Since the collision kernel (73) can be expressed as

$$\mathcal{B}_{\alpha\beta}(\boldsymbol{\xi}, \boldsymbol{\xi}_*, I, I_*, R, r, \sigma) = K_{\alpha\beta}k_{\alpha\beta}\tilde{\mathcal{B}}_{\alpha\beta}(|\mathbf{g}|, I, I_*, R, r), \tag{A10}$$

where

$$\begin{aligned} \tilde{\mathcal{B}}_{\alpha\beta}(|\mathbf{g}|, I, I_*, R, r) &= R^{\frac{\gamma_{\alpha\beta}}{2}}|\mathbf{g}|^{\gamma_{\alpha\beta}} \\ &\qquad + \eta\left(r(1 - R)\frac{I}{\sum_\alpha m_\alpha}\right)^{\frac{\gamma_{\alpha\beta}}{2}} + \eta\left((1 - r)(1 - R)\frac{I_*}{\sum_\alpha m_\alpha}\right)^{\frac{\gamma_{\alpha\beta}}{2}}, \end{aligned}$$

it is possible to pass to the center-of-mass reference frame with the unit Jacobian

$$\begin{aligned} \begin{pmatrix} \mathfrak{m}_\alpha \\ \mathfrak{P}_\alpha \\ \tilde{\mathfrak{e}}_\alpha \end{pmatrix} &= \sum_\beta W_\alpha W_\beta K_{\alpha\beta}k_{\alpha\beta}\int_{\Delta^2\times K}\begin{pmatrix} m_\alpha(\boldsymbol{\xi}' - \boldsymbol{\xi}) \\ m_\alpha\left(\left|\boldsymbol{\xi}'\right|^2 - |\boldsymbol{\xi}|^2\right) \\ I' - I \end{pmatrix} \\ &\qquad \times e^{-a_{\alpha\beta}\left|\mathbf{g}+\mathbf{b}_{\alpha\beta}\right|^2}e^{-c_{\alpha\beta}\left|\mathbf{G}+d_{\alpha\beta}\mathbf{g}+\mathbf{e}_{\alpha\beta}\right|^2}I^{a_\alpha}I_*^{a_\beta}e^{-V_\alpha I - V_\beta I_*} \\ &\qquad\qquad \times \tilde{\mathcal{B}}_{\alpha\beta}\,\psi_{\alpha\beta}\,\mathrm{d}R\,\mathrm{d}r\,\mathrm{d}\sigma\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I\,\mathrm{d}\mathbf{G}, \end{aligned}$$

where the test functions are expressed as in (A9). It is straightforward to perform the integration with respect to the angular variable $\sigma \in S^2$ by exploiting parity arguments. Additionally, it is easy to compute integral with respect to the velocity of the center of mass **G**, yielding

$$\begin{aligned} \begin{pmatrix} \mathfrak{m}_\alpha \\ \mathfrak{P}_\alpha \\ \tilde{\mathfrak{e}}_\alpha \end{pmatrix} &= \sum_\beta W_\alpha W_\beta K_{\alpha\beta}k_{\alpha\beta}(4\pi)\left(\frac{\pi}{c_{\alpha\beta}}\right)^{3/2} \\ &\qquad \int_{\Delta\times[0,\infty)\times[0,1]^2} e^{-a_{\alpha\beta}\left|\mathbf{g}+\mathbf{b}_{\alpha\beta}\right|^2}I^{a_\alpha}I_*^{a_\beta}e^{-V_\alpha I - V_\beta I_*} \\ &\quad \begin{pmatrix} -\mu_{\alpha\beta}\mathbf{g} \\ \mu_{\alpha\beta}\left(-\frac{m_\beta}{m_\alpha+m_\beta}(1 - R) + 2d_{\alpha\beta}\right)|\mathbf{g}|^2 + 2\frac{m_\beta}{m_\alpha+m_\beta}R(I + I_*) + 2\mu_{\alpha\beta}\mathbf{e}_{\alpha\beta}\cdot\mathbf{g} \\ r(1 - R)\left(\frac{\mu_{\alpha\beta}}{2}|\mathbf{g}|^2 + I_*\right) - (1 - r(1 - R))I \end{pmatrix} \\ &\qquad\qquad \times \tilde{\mathcal{B}}_{\alpha\beta}\,\psi_{\alpha\beta}\,\mathrm{d}R\,\mathrm{d}r\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I. \end{aligned} \tag{A11}$$

Denoting

$$\begin{aligned} \mathfrak{m}_{\alpha\beta} &= -\mu_{\alpha\beta}W_\alpha W_\beta K_{\alpha\beta}k_{\alpha\beta}(4\pi)\left(\frac{\pi}{c_{\alpha\beta}}\right)^{3/2} \\ &\qquad \times \int_{\Delta\times[0,\infty)\times[0,1]^2}\mathbf{g}\,e^{-a_{\alpha\beta}\left|\mathbf{g}+\mathbf{b}_{\alpha\beta}\right|^2}I^{a_\alpha}I_*^{a_\beta}e^{-V_\alpha I - V_\beta I_*}\,\tilde{\mathcal{B}}_{\alpha\beta}\,\psi_{\alpha\beta}\mathrm{d}R\,\mathrm{d}r\,\mathrm{d}I_*\,\mathrm{d}\mathbf{g}\,\mathrm{d}I, \end{aligned} \tag{A12}$$

the following relations hold,

$$\mathfrak{m}_\alpha = \sum_\beta \mathfrak{m}_{\alpha\beta}, \quad \mathfrak{P}_\alpha = \tilde{\mathfrak{P}}_\alpha - 2\sum_\beta \mathbf{e}_{\alpha\beta} \cdot \mathfrak{m}_{\alpha\beta},$$

where $\tilde{\mathfrak{P}}_\alpha$ will be introduced below. Therefore, instead of computing (A11), we calculate

$$\begin{aligned} \begin{pmatrix} \mathfrak{m}_\alpha \\ \tilde{\mathfrak{P}}_\alpha \\ \tilde{\mathfrak{e}}_\alpha \end{pmatrix} &= \sum_\beta W_\alpha W_\beta K_{\alpha\beta} k_{\alpha\beta} (4\pi) \left(\frac{\pi}{c_{\alpha\beta}} \right)^{3/2} \\ &\quad \times \int_{\Delta \times [0,\infty) \times [0,1]^2} e^{-a_{\alpha\beta} \left| \mathbf{g} + \mathbf{b}_{\alpha\beta} \right|^2} I^{a_\alpha} I_*^{a_\beta} e^{-V_\alpha I - V_\beta I_*} \\ &\quad \times \begin{pmatrix} -\mu_{\alpha\beta} \mathbf{g} \\ \mu_{\alpha\beta} \left(-\frac{m_\beta}{m_\alpha + m_\beta} (1-R) + 2 d_{\alpha\beta} \right) |\mathbf{g}|^2 + 2 \frac{m_\beta}{m_\alpha + m_\beta} R (I + I_*) \\ r(1-R) \left(\frac{\mu_{\alpha\beta}}{2} |\mathbf{g}|^2 + I_* \right) - (1 - r(1-R)) I \end{pmatrix} \\ &\quad \times \tilde{\mathcal{B}}_{\alpha\beta}\, \psi_{\alpha\beta}(R)\, \mathrm{d}R\, \mathrm{d}r\, \mathrm{d}I_*\, \mathrm{d}\mathbf{g}\, \mathrm{d}I. \end{aligned} \tag{A13}$$

It is then possible to pass to the spherical coordinates for the relative velocity $\mathbf{g}$, with zenith direction $\frac{\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta}{|\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta|}$ and azimuthal angle θ as the angle between $\mathbf{g}$ and $\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta$. Recalling the notation $\mathbf{b}_{\alpha\beta} = \boldsymbol{v}_\beta - \boldsymbol{v}_\alpha$ and denoting $A_{\alpha\beta} = 2a_{\alpha\beta} |\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta|$, we firstly define integrals $\mathcal{I}_1(|\mathbf{g}|)$ and $\mathcal{I}_2(|\mathbf{g}|)$,

$$\begin{aligned} \mathcal{I}_1(|\mathbf{g}|) &= \int_0^\pi e^{A_{\alpha\beta} |\mathbf{g}| \cos\theta} \sin\theta \mathrm{d}\theta = \frac{2}{A_{\alpha\beta} |\mathbf{g}|} \sinh\left(A_{\alpha\beta} |\mathbf{g}|\right), \\ \mathcal{I}_2(|\mathbf{g}|) &= \int_0^\pi \cos\theta\, e^{A_{\alpha\beta} |\mathbf{g}| \cos\theta} \sin\theta \mathrm{d}\theta \\ &= \frac{2}{A_{\alpha\beta}^2 |\mathbf{g}|^2} \left(A_{\alpha\beta} |\mathbf{g}| \cosh\left(A_{\alpha\beta} |\mathbf{g}|\right) - \sinh\left(A_{\alpha\beta} |\mathbf{g}|\right) \right) \\ &= \frac{A_{\alpha\beta} \sqrt{\pi}}{2} |\mathbf{g}|\, {}_0\tilde{F}_1 \left(\frac{5}{2}, \frac{A_{\alpha\beta}^2}{4} |\mathbf{g}|^2 \right), \end{aligned} \tag{A14}$$

where the regularized hypergeometric function ${}_0\tilde{F}_1$ defined in (A5) is used. This allows us to pass to the spherical coordinates for $\mathbf{g}$ and rewrite integrals appearing in (A13) in a suitable form involving the notation (76), for some $y \geq 0$,

$$\begin{aligned} &\int_{\mathbb{R}^3} e^{-a_{\alpha\beta} \left| \mathbf{g} + \mathbf{b}_{\alpha\beta} \right|^2} |\mathbf{g}|^y \mathrm{d}\mathbf{g} = 2\pi e^{-a_{\alpha\beta} \left| \boldsymbol{v}_\alpha - \boldsymbol{v}_\beta \right|^2} \int_{[0,\infty)} e^{-a_{\alpha\beta} |\mathbf{g}|^2} |\mathbf{g}|^{y+2} \mathcal{I}_1(|\mathbf{g}|) \mathrm{d}|\mathbf{g}| \\ &= \pi^{3/2} e^{-a_{\alpha\beta} \left| \boldsymbol{v}_\alpha - \boldsymbol{v}_\beta \right|^2} a_{\alpha\beta}^{-\frac{y+3}{2}}\, \Gamma\left(\tfrac{y+3}{2} \right) {}_1\tilde{F}_1 \left(\tfrac{y+3}{2}, \tfrac{3}{2}, a_{\alpha\beta} \left| \boldsymbol{v}_\alpha - \boldsymbol{v}_\beta \right|^2 \right) =: \left(\frac{\pi}{a_{\alpha\beta}} \right)^{3/2} \mathcal{F}_y^1. \end{aligned} \tag{A15}$$

Note that for $y = 2$ and $y = 0$ this integral simplifies to

$$\mathcal{F}_2^1 = \frac{3}{2} a_{\alpha\beta}^{-1} + \left| \boldsymbol{v}_\alpha - \boldsymbol{v}_\beta \right|^2, \quad \mathcal{F}_0^1 = 1. \tag{A16}$$

On the other side, for the term involving $\mathcal{I}_2$, parity arguments imply

$$
\begin{aligned}
&\int_{\mathbb{R}^3} \mathbf{g}\,|\mathbf{g}|^y e^{-a_{\alpha\beta}|\mathbf{g}+\mathbf{b}_{\alpha\beta}|^2}\mathrm{d}\mathbf{g}\\
&\qquad = 2\pi e^{-a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2}\,\frac{\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta}{|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|}\int_{[0,\infty)} e^{-a_{\alpha\beta}|\mathbf{g}|^2}|\mathbf{g}|^{y+3}\mathcal{I}_2(|\mathbf{g}|)\mathrm{d}|\mathbf{g}|\\
&\qquad = \pi^{3/2}e^{-a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2}(\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta)\,a_{\alpha\beta}^{-\frac{y+3}{2}}\,\Gamma\Big(\tfrac{y+5}{2}\Big)\,{}_1\tilde{F}_1\Big(\tfrac{y+5}{2},\tfrac{5}{2},a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2\Big)\\
&\qquad =: (\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta)\left(\frac{\pi}{a_{\alpha\beta}}\right)^{3/2}\mathcal{F}_y^2,
\end{aligned}
\tag{A17}
$$

where the hypergeometric function ${}_1\tilde{F}_1$ is defined in (A6). Note $\mathcal{F}_0^2 = 1$.

Therefore, using angular integrals (A14), production terms (A13) can be simplified to

$$
\begin{aligned}
\begin{pmatrix}\mathfrak{m}_\alpha\\ \tilde{\mathfrak{P}}_\alpha\\ \tilde{\mathfrak{e}}_\alpha\end{pmatrix} &= \sum_\beta W_\alpha W_\beta K_{\alpha\beta}(8\pi^2)\left(\frac{\pi}{c_{\alpha\beta}}\right)^{3/2} e^{-a_{\alpha\beta}|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|^2}\\
&\qquad \int_{[0,\infty)^3\times[0,1]^2}|\mathbf{g}|^2 e^{-a_{\alpha\beta}|\mathbf{g}|^2} I^{a_\alpha} I_*^{a_\beta} e^{-V_\alpha I - V_\beta I_*}\\
&\times\begin{pmatrix} -\mu_{\alpha\beta}|\mathbf{g}|\mathcal{I}_2(|\mathbf{g}|)\frac{\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta}{|\boldsymbol{v}_\alpha-\boldsymbol{v}_\beta|}\\ \Big(\mu_{\alpha\beta}\Big(-\frac{m_\beta}{m_\alpha+m_\beta}(1-R)+2d_{\alpha\beta}\Big)|\mathbf{g}|^2+2\frac{m_\beta}{m_\alpha+m_\beta}R(I+I_*)\Big)\mathcal{I}_1(|\mathbf{g}|)\\ \Big(r(1-R)\Big(\frac{\mu_{\alpha\beta}}{2}|\mathbf{g}|^2+I_*\Big)-(1-r(1-R))I\Big)\mathcal{I}_1(|\mathbf{g}|)\end{pmatrix}\\
&\qquad\qquad \times\tilde{\mathcal{B}}_{\alpha\beta}\,\psi_{\alpha\beta}\,\mathrm{d}R\,\mathrm{d}r\,\mathrm{d}I_*\,\mathrm{d}I\,\mathrm{d}|\mathbf{g}|.
\end{aligned}
\tag{A18}
$$

Further computations can be done only by specifying $\tilde{\mathcal{B}}_{\alpha\beta}$ from (A10) and expanding all terms. Then, it will be possible to specify y in (76) from integration with respect to $|\mathbf{g}|$ and perform integration with respect to I and I_* using

$$
\begin{aligned}
B_{(a,b)} &= \frac{V_\alpha^{a_\alpha+1}}{\Gamma(a_\alpha+1)}\frac{V_\beta^{a_\beta+1}}{\Gamma(a_\beta+1)}\int_{[0,\infty)^2} I^{a_\alpha+a} I_*^{a_\beta+b} e^{-V_\alpha I - V_\beta I_*}\mathrm{d}I_*\,\mathrm{d}I\\
&= V_\alpha^{-a}V_\beta^{-b}\frac{\Gamma(a_\alpha+a+1)\Gamma(a_\beta+b+1)}{\Gamma(a_\alpha+1)\Gamma(a_\beta+1)},
\end{aligned}
\tag{A19}
$$

as much as the integration with respect to the variables $r, R \in [0,1]$ introducing

$$
\begin{aligned}
C_{(a,b,c,d)} &= k_{\alpha\beta}\int_{[0,1]^2}(1-R)^a R^b r^c (1-r)^d\,\psi_{\alpha\beta}(r,R)\mathrm{d}r\,\mathrm{d}R\\
&= k_{\alpha\beta}\frac{\Gamma\big(a_\alpha+a_\beta+a+2\big)\Gamma\big(b+\frac{3}{2}\big)\Gamma(a_\alpha+c+1)\Gamma\big(a_\beta+d+1\big)}{\Gamma\big(a_\alpha+a_\beta+a+b+\frac{7}{2}\big)\Gamma\big(a_\alpha+a_\beta+c+d+2\big)},
\end{aligned}
\tag{A20}
$$

Therefore, in what follows, we consider each production term separately.

Appendix C.1. Production Term $\mathfrak{m}_\alpha$

Using the notations (A19) and (A20), the production term $\mathfrak{m}_\alpha$ becomes

$$
\begin{aligned}
\mathfrak{m}_\alpha = -\sum_\beta \frac{\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta}{|\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta|} \frac{\rho_\alpha}{m_\alpha} \frac{\rho_\beta}{m_\beta} K_{\alpha\beta} (8\sqrt{\pi}) \left(\frac{U_\alpha U_\beta}{c_{\alpha\beta}} \right)^{3/2} & e^{-a_{\alpha\beta} |\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta|^2} \mu_{\alpha\beta} \\
\times \int_{[0,\infty)} \mathcal{I}_2(|\mathbf{g}|) |\mathbf{g}|^3 e^{-a_{\alpha\beta}|\mathbf{g}|^2} \Big\{ C_{\left(0,\frac{\gamma_{\alpha\beta}}{2},0,0\right)} |\mathbf{g}|^{\gamma_{\alpha\beta}} & \\
+ \eta \Big(\sum_\alpha m_\alpha \Big)^{-\gamma_{\alpha\beta}/2} \left(B_{\left(\frac{\gamma_{\alpha\beta}}{2},0\right)} C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)} + B_{\left(0,\frac{\gamma_{\alpha\beta}}{2}\right)} C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)} \right) & \Big\} \mathrm{d}|\mathbf{g}|.
\end{aligned}
$$

Using (A17) and $U_\alpha U_\beta (a_{\alpha\beta} c_{\alpha\beta})^{-1} = 1$,

$$
\begin{aligned}
\mathfrak{m}_\alpha = -\sum_\beta (\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta) \frac{\rho_\alpha}{m_\alpha} \frac{\rho_\beta}{m_\beta} K_{\alpha\beta} (4\pi) \mu_{\alpha\beta} \Big\{ & C_{\left(0,\frac{\gamma_{\alpha\beta}}{2},0,0\right)} \mathcal{F}^2_{\gamma_{\alpha\beta}} \\
& + \eta \Big(\sum_\alpha m_\alpha \Big)^{-\gamma_{\alpha\beta}/2} \left(B_{\left(\frac{\gamma_{\alpha\beta}}{2},0\right)} C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)} + B_{\left(0,\frac{\gamma_{\alpha\beta}}{2}\right)} C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)} \right) \Big\}.
\end{aligned}
$$

Expanding constants (A19) and (A20) and simplifying expressions involving Gamma functions yield the final expression (78).

Appendix C.2. Production Term $\tilde{\mathfrak{P}}_\alpha$

Using the notation for constants (A19) and (A20), the production term $\tilde{\mathfrak{P}}_\alpha$ becomes

$$
\begin{aligned}
\tilde{\mathfrak{P}}_\alpha = & \sum_\beta \frac{\rho_\alpha}{m_\alpha} \frac{\rho_\beta}{m_\beta} K_{\alpha\beta} (8\sqrt{\pi}) \left(\frac{U_\alpha U_\beta}{c_{\alpha\beta}} \right)^{3/2} e^{-a_{\alpha\beta} |\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta|^2} \int_{[0,\infty)} \mathcal{I}_1(|\mathbf{g}|) |\mathbf{g}|^2 e^{-a_{\alpha\beta}|\mathbf{g}|^2} \\
\times & \Bigg(|\mathbf{g}|^{2+\gamma_{\alpha\beta}} \mu_{\alpha\beta} \left(-\frac{m_\beta}{m_\alpha + m_\beta} C_{\left(1,\frac{\gamma_{\alpha\beta}}{2},0,0\right)} + 2 d_{\alpha\beta} C_{\left(0,\frac{\gamma_{\alpha\beta}}{2},0,0\right)} \right) \\
& + |\mathbf{g}|^{\gamma_{\alpha\beta}} \frac{2 m_\beta}{m_\alpha + m_\beta} C_{\left(0,1+\frac{\gamma_{\alpha\beta}}{2},0,0\right)} \left(B_{(1,0)} + B_{(0,1)} \right) \\
& + \frac{\eta\, \mu_{\alpha\beta} |\mathbf{g}|^2}{(\sum_\alpha m_\alpha)^{\frac{\gamma_{\alpha\beta}}{2}}} \Bigg(\left(-\frac{m_\beta}{m_\alpha + m_\beta} C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)} + 2 d_{\alpha\beta} C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)} \right) B_{\left(\frac{\gamma_{\alpha\beta}}{2},0\right)} \\
& \qquad + \left(-\frac{m_\beta}{m_\alpha + m_\beta} C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)} + 2 d_{\alpha\beta} C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)} \right) B_{\left(0,\frac{\gamma_{\alpha\beta}}{2}\right)} \Bigg) \\
& + \frac{2 m_\beta}{m_\alpha + m_\beta} \frac{\eta}{(\sum_\alpha m_\alpha)^{\frac{\gamma_{\alpha\beta}}{2}}} \Bigg(C_{\left(\frac{\gamma_{\alpha\beta}}{2},1,\frac{\gamma_{\alpha\beta}}{2},0\right)} \left(B_{\left(\frac{\gamma_{\alpha\beta}}{2}+1,0\right)} + B_{\left(\frac{\gamma_{\alpha\beta}}{2},1\right)} \right) \\
& \qquad + C_{\left(\frac{\gamma_{\alpha\beta}}{2},1,0,\frac{\gamma_{\alpha\beta}}{2}\right)} \left(B_{\left(1,\frac{\gamma_{\alpha\beta}}{2}\right)} + B_{\left(\frac{\gamma_{\alpha\beta}}{2}+1\right)} \right) \Bigg) \Bigg) \mathrm{d}|\mathbf{g}|.
\end{aligned}
$$

Involving (A15), integration with respect to $|\mathbf{g}|$ yields

$$
\begin{aligned}
\tilde{\mathfrak{P}}_\alpha = {} & \sum_\beta \frac{\rho_\alpha}{m_\alpha}\frac{\rho_\beta}{m_\beta}K_{\alpha\beta}(4\pi) \\
\times & \Bigg(\mathcal{F}^2_{2+\gamma_{\alpha\beta}}\mu_{\alpha\beta}\left(-\frac{m_\beta}{m_\alpha+m_\beta}C_{\left(1,\frac{\gamma_{\alpha\beta}}{2},0,0\right)}+2d_{\alpha\beta}C_{\left(0,\frac{\gamma_{\alpha\beta}}{2},0,0\right)}\right) \\
& +\mathcal{F}^2_{\gamma_{\alpha\beta}}\frac{2m_\beta}{m_\alpha+m_\beta}C_{\left(0,1+\frac{\gamma_{\alpha\beta}}{2},0,0\right)}\left(B_{(1,0)}+B_{(0,1)}\right) \\
& +\frac{\eta\,\mu_{\alpha\beta}\mathcal{F}^2_2}{\left(\sum_\alpha m_\alpha\right)^{\frac{\gamma_{\alpha\beta}}{2}}}\Bigg(\left(-\frac{m_\beta}{m_\alpha+m_\beta}C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)}+2d_{\alpha\beta}C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)}\right)B_{\left(\frac{\gamma_{\alpha\beta}}{2},0\right)} \\
& \qquad +\left(-\frac{m_\beta}{m_\alpha+m_\beta}C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)}+2d_{\alpha\beta}C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)}\right)B_{\left(0,\frac{\gamma_{\alpha\beta}}{2}\right)}\Bigg) \\
& +\frac{2m_\beta}{m_\alpha+m_\beta}\frac{\eta}{\left(\sum_\alpha m_\alpha\right)^{\frac{\gamma_{\alpha\beta}}{2}}}\Bigg(C_{\left(\frac{\gamma_{\alpha\beta}}{2},1,\frac{\gamma_{\alpha\beta}}{2},0\right)}\left(B_{\left(\frac{\gamma_{\alpha\beta}}{2}+1,0\right)}+B_{\left(\frac{\gamma_{\alpha\beta}}{2},1\right)}\right) \\
& \qquad +C_{\left(\frac{\gamma_{\alpha\beta}}{2},1,0,\frac{\gamma_{\alpha\beta}}{2}\right)}\left(B_{\left(1,\frac{\gamma_{\alpha\beta}}{2}\right)}+B_{\left(\frac{\gamma_{\alpha\beta}}{2}+1\right)}\right)\Bigg)\Bigg).
\end{aligned}
$$

The expansion of coefficients B and C using their definitions (A19) and (A20) yields the final expression (80).

Appendix C.3. Production Term $\tilde{\mathfrak{e}}_\alpha$

In the similar fashion, the production term $\tilde{\mathfrak{e}}_\alpha$ becomes

$$
\begin{aligned}
\tilde{\mathfrak{e}}_\alpha = {} & \sum_\beta \frac{\rho_\alpha}{m_\alpha}\frac{\rho_\beta}{m_\beta}K_{\alpha\beta}(4\pi)\Bigg(\frac{\mu_{\alpha\beta}}{2}\mathcal{F}^1_{2+\gamma_{\alpha\beta}}C_{\left(1,\frac{\gamma_{\alpha\beta}}{2},1,0\right)} \\
& +\mathcal{F}^1_{\gamma_{\alpha\beta}}\left(B_{(0,1)}C_{\left(1,\frac{\gamma_{\alpha\beta}}{2},1,0\right)}-B_{(1,0)}\left(C_{\left(0,\frac{\gamma_{\alpha\beta}}{2},0,0\right)}-C_{\left(1,\frac{\gamma_{\alpha\beta}}{2},1,0\right)}\right)\right) \\
& +\frac{\mu_{\alpha\beta}}{2\left(\sum_\alpha m_\alpha\right)^{\frac{\gamma_{\alpha\beta}}{2}}}\mathcal{F}^1_2\left(B_{\left(\frac{\gamma_{\alpha\beta}}{2},0\right)}C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,1+\frac{\gamma_{\alpha\beta}}{2},0\right)}+B_{\left(0,\frac{\gamma_{\alpha\beta}}{2}\right)}C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,1,\frac{\gamma_{\alpha\beta}}{2}\right)}\right) \\
& +\frac{\eta}{\left(\sum_\alpha m_\alpha\right)^{\frac{\gamma_{\alpha\beta}}{2}}}\Bigg\{B_{\left(\frac{\gamma_{\alpha\beta}}{2},1\right)}C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,1+\frac{\gamma_{\alpha\beta}}{2},0\right)}+B_{\left(0,1+\frac{\gamma_{\alpha\beta}}{2}\right)}C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,1,\frac{\gamma_{\alpha\beta}}{2}\right)} \\
& \qquad -B_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0\right)}\left(C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,\frac{\gamma_{\alpha\beta}}{2},0\right)}-C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,1+\frac{\gamma_{\alpha\beta}}{2},0\right)}\right) \\
& \qquad -B_{\left(1,\frac{\gamma_{\alpha\beta}}{2}\right)}\left(C_{\left(\frac{\gamma_{\alpha\beta}}{2},0,0,\frac{\gamma_{\alpha\beta}}{2}\right)}-C_{\left(1+\frac{\gamma_{\alpha\beta}}{2},0,1,\frac{\gamma_{\alpha\beta}}{2}\right)}\right)\Bigg\}\Bigg).
\end{aligned}
$$

After expanding constants, we get the final expression (81).

Appendix D. Linearization of Source Terms

We first introduce the following notation, common to all production terms,

$$
\begin{aligned}
\mathfrak{h}_1 &= \frac{2}{\sqrt{\pi}}\Gamma\!\left(\tfrac{\gamma_{\alpha\beta}+3}{2}\right)\Gamma\!\left(\tfrac{\gamma_{\alpha\beta}+5}{2}\right)\frac{k_B}{(m_\alpha+m_\beta)}\left(\frac{2k_B}{\mu_{\alpha\beta}}\right)^{\gamma_{\alpha\beta}/2}, \\
\mathfrak{h}_2 &= \eta\frac{k_B^{1+\gamma_{\alpha\beta}/2}}{(m_\alpha+m_\beta)}.
\end{aligned}
\tag{A21}
$$

Appendix D.1. Production Term $\mathfrak{m}_\alpha$

In order to linearize the production term $\mathfrak{m}_\alpha$, we compute the gradient. In this case, the only term that does not vanish in the equilibrium state w^0 for equal velocities, temperatures, and vanishing dynamic pressure is the term related to velocities, i.e., for any $i, j = 1, \ldots, 3$,

$$\begin{aligned} \frac{\partial \mathfrak{m}_{\alpha\beta i}}{\partial v_{\alpha j}}(w^0) &= -\frac{\partial \mathfrak{m}_{\alpha\beta i}}{\partial v_{\beta j}}(w^0) \\ &= -\delta_{ij}\,\frac{m_\alpha m_\beta}{k_B}\Big(a_\alpha + a_\beta + \tfrac{\gamma_{\alpha\beta}+7}{2}\Big)\Big(\frac{2}{3}\mathfrak{h}_1 + \mathfrak{h}_2(\mathcal{C}_\alpha + \mathcal{C}_\beta)\Big)T^{\frac{\gamma_{\alpha\beta}}{2}}. \end{aligned} \tag{A22}$$

Therefore, the production term $\mathfrak{m}_\alpha$, can be approximated as stated in (82),

$$\mathfrak{m}_\alpha \approx -\sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{n} \mathcal{M}_{\alpha\beta}\,\rho_\alpha\rho_\beta\,(\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta)\,T^{\frac{\gamma_{\alpha\beta}}{2}},$$

where the constant $\mathcal{M}_{\alpha\beta}$, non-negative and symmetric in (α, β), is given by

$$\mathcal{M}_{\alpha\beta} = \mathcal{K}_{\alpha\beta}\frac{m_\alpha m_\beta}{k_B}\Big(a_\alpha + a_\beta + \tfrac{\gamma_{\alpha\beta}+7}{2}\Big)\Big(\frac{2}{3}\mathfrak{h}_1 + \mathfrak{h}_2(\mathcal{C}_\alpha + \mathcal{C}_\beta)\Big), \tag{A23}$$

with notation (A21).

Appendix D.2. Production Term $\mathfrak{P}_\alpha$

From the expression for the production term $\mathfrak{P}_\alpha$ given in (79), we can compute its gradient,

$$\nabla\mathfrak{P}_\alpha(w^0) = \sum_{\beta=1}^{n} \rho_\alpha\rho_\beta\,\mathcal{K}_{\alpha\beta}\Big(\nabla\tilde{\mathfrak{P}}_{\alpha\beta}(w^0) + 2v_i\nabla\mathfrak{m}_{\alpha\beta i}(w^0)\Big),$$

Then we compute derivatives of $\tilde{\mathfrak{P}}_{\alpha\beta}$ and evaluate at the equilibrium state w^0,

$$\begin{aligned} \frac{\partial\tilde{\mathfrak{P}}_{\alpha\beta}}{\partial T_\alpha}(w^0) &= -\frac{\partial\tilde{\mathfrak{P}}_{\alpha\beta}}{\partial T_\beta}(w^0) = m_\beta\Big(\tfrac{1}{(m_\alpha+m_\beta)}\mathfrak{h}_1 c_1 + 3\,\mathfrak{h}_2 c_2\Big)T^{\frac{\gamma_{\alpha\beta}}{2}}, \\ \frac{\partial\tilde{\mathfrak{P}}_{\alpha\beta}}{\partial\Pi_\alpha}(w^0) &= \frac{m_\beta}{k_B\,n_\alpha}\Big(\tfrac{1}{(m_\alpha+m_\beta)}\mathfrak{h}_1 c_3 + 3\,\mathfrak{h}_2 c_4\Big)T^{\frac{\gamma_{\alpha\beta}}{2}}, \\ \frac{\partial\tilde{\mathfrak{P}}_{\alpha\beta}}{\partial\Pi_\beta}(w^0) &= \frac{m_\beta}{k_B\,n_\beta}\Big(\tfrac{1}{(m_\alpha+m_\beta)}\mathfrak{h}_1 c_5 + 3\,\mathfrak{h}_2 c_6\Big)T^{\frac{\gamma_{\alpha\beta}}{2}}, \end{aligned} \tag{A24}$$

where the constants are

$$\begin{aligned} c_1 &= 2\big(m_\alpha\big(a_\alpha + 2a_\beta + 6 + \gamma_{\alpha\beta}\big) + \big(a_\beta + 1\big)m_\beta\big) > 0, \\ c_2 &= \frac{c_1}{2(m_\alpha + m_\beta)}(\mathcal{C}_\alpha + \mathcal{C}_\beta) + \frac{\gamma_{\alpha\beta}}{2(m_\alpha + m_\beta)}(m_\beta\mathcal{C}_\beta - m_\alpha\mathcal{C}_\alpha) > 0, \\ c_3 &= c_1 + (m_\alpha + m_\beta)(2a_\alpha + 5) > 0, \\ c_4 &= c_2 + \left(a_\alpha + \frac{5}{2}\right)\left(\left(1 + \frac{\gamma_{\alpha\beta}}{2(a_\alpha + 1)}\right)\mathcal{C}_\alpha + \mathcal{C}_\beta\right) > 0, \\ c_5 &= c_1 - (m_\alpha + m_\beta)(2a_\beta + 5), \\ c_6 &= c_2 - \left(a_\beta + \frac{5}{2}\right)\left(\mathcal{C}_\alpha + \left(1 + \frac{\gamma_{\alpha\beta}}{2(a_\beta + 1)}\right)\mathcal{C}_\beta\right), \end{aligned}$$

where the involved constants are given in (75). Therefore, taking into account (A22) and (A24), the production term $\mathfrak{P}_\alpha$ can be approximated as

$$
\begin{aligned}
\mathfrak{P}_\alpha \approx \sum_{\beta=1}^{n} \rho_\alpha \rho_\beta \, \mathcal{K}_{\alpha\beta} \\
\times \Bigg(- \boldsymbol{v} \cdot (\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta) T^{\frac{\gamma_{\alpha\beta}}{2}} \frac{2 m_\alpha m_\beta}{k_B} \left(a_\alpha + a_\beta + \tfrac{\gamma_{\alpha\beta}+7}{2} \right) \left(\frac{2}{3} \mathfrak{h}_1 + \mathfrak{h}_2 (\mathcal{C}_\alpha + \mathcal{C}_\beta) \right) \\
- m_\beta \left(\tfrac{1}{(m_\alpha + m_\beta)} \mathfrak{h}_1 c_1 + 3 \, \mathfrak{h}_2 c_2 \right) T^{\frac{\gamma_{\alpha\beta}}{2}} (T_\alpha - T_\beta) \\
- m_\beta \left(\tfrac{1}{(m_\alpha + m_\beta)} \mathfrak{h}_1 c_3 + 3 \, \mathfrak{h}_2 c_4 \right) T^{\frac{\gamma_{\alpha\beta}}{2}} \frac{\Pi_\alpha}{k_B \, n_\alpha} + m_\beta \left(\tfrac{1}{(m_\alpha + m_\beta)} \mathfrak{h}_1 c_5 + 3 \, \mathfrak{h}_2 c_6 \right) T^{\frac{\gamma_{\alpha\beta}}{2}} \frac{\Pi_\beta}{k_B \, n_\beta} \Bigg),
\end{aligned}
$$

which is exactly (83) with notation (A23) and

$$
\begin{aligned}
\mathcal{P}^{T}_{\alpha\beta} &= m_\beta \, \mathcal{K}_{\alpha\beta} \left(\tfrac{1}{(m_\alpha + m_\beta)} \mathfrak{h}_1 c_1 + 3 \, \mathfrak{h}_2 c_2 \right) > 0, \\
\mathcal{P}^{\Pi}_{\alpha\beta} &= m_\beta \, \mathcal{K}_{\alpha\beta} \left(\tfrac{1}{(m_\alpha + m_\beta)} \mathfrak{h}_1 c_3 + 3 \, \mathfrak{h}_2 c_4 \right) > 0, \\
\tilde{\mathcal{P}}^{\Pi}_{\alpha\beta} &= m_\beta \, \mathcal{K}_{\alpha\beta} \left(\tfrac{1}{(m_\alpha + m_\beta)} \mathfrak{h}_1 c_5 + 3 \, \mathfrak{h}_2 c_6 \right).
\end{aligned}
\tag{A25}
$$

The following combination of the aforementioned constants is used

$$
\begin{aligned}
\frac{\mathcal{P}^{\Pi}_{bc} \tilde{A}_c - \tilde{\mathcal{P}}^{\Pi}_{bc} \tilde{A}_b}{A_b \tilde{A}_c - A_c \tilde{A}_b} &= \frac{(\tilde{A}_c - \tilde{A}_b) \mathcal{P}^{T}_{bc} + m_c \, \mathcal{P}^{\chi}_{bc}}{A_b \tilde{A}_c - A_c \tilde{A}_b} \\
&= -2 \left(\mathcal{P}^{T}_{bc} + \frac{2 \, m_c (1 + a_b)(1 + a_c)}{3 (a_b - a_c)} \mathcal{P}^{\chi}_{bc} \right),
\end{aligned}
\tag{A26}
$$

where $\mathcal{P}^{\chi}_{bc}$ is positive and symmetric in (b, c) and is given by

$$
\begin{aligned}
\mathcal{P}^{\chi}_{bc} = \tfrac{3}{2} \mathcal{K}_{bc} \Bigg(\mathfrak{h}_1 \left(\frac{2 a_b + 5}{a_c + 1} + \frac{2 a_c + 5}{a_b + 1} \right) \\
+ 3 \, \mathfrak{h}_2 \Bigg\{ \left(\frac{a_b + \frac{5}{2}}{a_c + 1} \right) \left(\left(1 + \frac{\gamma_{\alpha\beta}}{2 (a_b + 1)} \right) \mathcal{C}_b + \mathcal{C}_c \right) \\
+ \left(\frac{a_c + \frac{5}{2}}{a_b + 1} \right) \left(\left(1 + \frac{\gamma_{\alpha\beta}}{2 (a_c + 1)} \right) \mathcal{C}_c + \mathcal{C}_b \right) \Bigg\} \Bigg),
\end{aligned}
\tag{A27}
$$

as much as

$$
\frac{1}{A_b A_n} \left[(\tilde{A}_b A_n - \tilde{A}_n A_b) \mathcal{P}^{T}_{bn} + \mathcal{P}^{\Pi}_{bn} A_n - \tilde{\mathcal{P}}^{\Pi}_{bn} A_b \right] = m_n \mathcal{P}^{\omega}_{bn},
\tag{A28}
$$

with $\mathcal{P}^{\omega}_{bn} > 0$ given by

$$
\mathcal{P}^{\omega}_{bn} = \mathcal{K}_{bn} (4 (2 + a_b + a_n) \mathfrak{h}_1 + 3 (\gamma_{bn} + 2 (2 + a_b + a_n)) (\mathcal{C}_b + \mathcal{C}_n) \mathfrak{h}_2),
\tag{A29}
$$

where $\mathfrak{h}_1$ and $\mathfrak{h}_2$ are to be understood as (A21) for $\alpha = b$ and $\beta = n$.

Appendix D.3. Production Term $\mathfrak{e}_\alpha$

Taking into account (68), the gradient of $\mathfrak{e}_\alpha$ at the equilibrium state w^0 can be computed as

$$
\nabla \mathfrak{e}_\alpha (w^0) = \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^{n} \rho_\alpha \rho_\beta \, \mathcal{K}_{\alpha\beta} \left(\frac{\nabla \mathfrak{P}_{\alpha\beta} (w^0)}{2} + \nabla \tilde{\mathfrak{e}}_{\alpha\beta} (w^0) \right).
$$

Derivatives of $\tilde{\mathfrak{e}}_{\alpha\beta}$ evaluated at w^0 are given as follows

$$\frac{\partial \tilde{\mathfrak{e}}_{\alpha\beta}}{\partial T_\alpha}(w^0) = -\frac{\partial \tilde{\mathfrak{e}}_{\alpha\beta}}{\partial T_\beta}(w^0) = \left(\tfrac{a_\alpha+1}{\gamma_{\alpha\beta}+3}\,\mathfrak{h}_1\tilde{c}_1 + \mathfrak{h}_2\tilde{c}_2\right)T^{\frac{\gamma_{\alpha\beta}}{2}},$$

$$\frac{\partial \tilde{\mathfrak{e}}_{\alpha\beta}}{\partial \Pi_\alpha}(w^0) = \frac{T^{\frac{\gamma_{\alpha\beta}}{2}}}{k_B\,n_\alpha}\left(\tfrac{a_\alpha+1}{\gamma_{\alpha\beta}+3}\,\mathfrak{h}_1\tilde{c}_3 + \mathfrak{h}_2\tilde{c}_4\right), \quad \frac{\partial \tilde{\mathfrak{e}}_{\alpha\beta}}{\partial \Pi_\beta}(w^0) = \frac{T^{\frac{\gamma_{\alpha\beta}}{2}}}{k_B\,n_\beta}\left(\tfrac{a_\alpha+1}{\gamma_{\alpha\beta}+3}\,\mathfrak{h}_1\tilde{c}_5 + \mathfrak{h}_2\tilde{c}_6\right),$$

where the involved terms are defined as

$$\begin{aligned}
\tilde{c}_1 &= -m_\alpha\big(\gamma_{\alpha\beta} + 2a_\beta + 5\big) - 2\big(a_\beta + 1\big)m_\beta,\\
\tilde{c}_2 &= \frac{a_\alpha + 1}{2}\left(\tilde{c}_1\left[\left(1 + \frac{\gamma_{\alpha\beta}}{2(a_\alpha+1)}\right)\mathcal{C}_\alpha + \mathcal{C}_\beta\right]\right.\\
&\qquad\left. + \gamma_{\alpha\beta}\left[\left(1 + \frac{\gamma_{\alpha\beta}}{2(a_\alpha+1)}\right)m_\alpha\mathcal{C}_\alpha - m_\beta\mathcal{C}_\beta\right]\right),\\
\tilde{c}_3 &= \frac{1}{2(a_\alpha+1)}\big(-3\,\tilde{c}_1 + m_\beta\big(\gamma_{\alpha\beta}+3\big)\big(2a_\alpha+5\big)\big)\\
\tilde{c}_4 &= -\frac{3}{2(a_\alpha+1)}\tilde{c}_2 + \frac{3}{4}(2a_\alpha+5)m_\beta\left(\frac{\big(2a_\alpha + \gamma_{\alpha\beta} + 2\big)}{2(a_\alpha+1)}\mathcal{C}_\alpha + \mathcal{C}_\beta\right)\\
\tilde{c}_5 &= \gamma_{\alpha\beta}\,m_\alpha - 3m_\beta,\\
\tilde{c}_6 &= -\tilde{c}_2 - \frac{\big(2a_\beta+5\big)\big(m_\alpha+m_\beta\big)}{4\big(a_\beta+1\big)}\Big(\big(a_\beta+1\big)\big(2a_\alpha+\gamma_{\alpha\beta}+2\big)\mathcal{C}_\alpha\\
&\qquad + \big(a_\alpha+1\big)\big(\gamma_{\alpha\beta}+2a_\beta+2\big)\mathcal{C}_\beta\Big).
\end{aligned}$$

Therefore, $\tilde{\mathfrak{e}}_{\alpha\beta}$ can be linearized as follows

$$\begin{aligned}
\tilde{\mathfrak{e}}_{\alpha\beta} \approx{}& \left(\tfrac{a_\alpha+1}{\gamma_{\alpha\beta}+3}\,\mathfrak{h}_1\tilde{c}_1 + \mathfrak{h}_2\tilde{c}_2\right)T^{\frac{\gamma_{\alpha\beta}}{2}}\left(T_\alpha - T_\beta\right)\\
&+ \frac{\Pi_\alpha}{k_B\,n_\alpha}T^{\frac{\gamma_{\alpha\beta}}{2}}\left(\tfrac{a_\alpha+1}{\gamma_{\alpha\beta}+3}\,\mathfrak{h}_1\tilde{c}_3 + \mathfrak{h}_2\tilde{c}_4\right) + \frac{\Pi_\beta}{k_B\,n_\beta}T^{\frac{\gamma_{\alpha\beta}}{2}}\left(\tfrac{a_\alpha+1}{\gamma_{\alpha\beta}+3}\,\mathfrak{h}_1\tilde{c}_5 + \mathfrak{h}_2\tilde{c}_6\right).
\end{aligned} \tag{A30}$$

Combining the last expression with (83), $\mathfrak{e}_\alpha$ can be approximated as

$$\begin{aligned}
\mathfrak{e}_\alpha \approx{}& \sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{n} \rho_\alpha\rho_\beta\,\mathcal{K}_{\alpha\beta}\\
&\times\left(-\,\boldsymbol{v}\cdot\left(\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta\right)T^{\frac{\gamma_{\alpha\beta}}{2}}\frac{m_\alpha m_\beta}{k_B}\left(a_\alpha + a_\beta + \tfrac{\gamma_{\alpha\beta}+7}{2}\right)\left(\frac{2}{3}\mathfrak{h}_1 + \mathfrak{h}_2\big(\mathcal{C}_\alpha + \mathcal{C}_\beta\big)\right)\right.\\
&\quad - \Big(\mathfrak{h}_1\left[\hat{c}_1(\alpha,\beta) + \hat{c}_1(\beta,\alpha)\right] + \mathfrak{h}_2\left[\hat{c}_2(\alpha,\beta) + \hat{c}_2(\beta,\alpha)\right]\Big)T^{\frac{\gamma_{\alpha\beta}}{2}}\left(T_\alpha - T_\beta\right)\\
&\left. + \left(\mathfrak{h}_1\hat{c}_3(\alpha,\beta) + \mathfrak{h}_2\,\hat{c}_4(\alpha,\beta)\right)T^{\frac{\gamma_{\alpha\beta}}{2}}\frac{\Pi_\alpha}{k_B\,n_\alpha} - \left(\mathfrak{h}_1\hat{c}_3(\beta,\alpha) + \mathfrak{h}_2\,\hat{c}_4(\beta,\alpha)\right)T^{\frac{\gamma_{\alpha\beta}}{2}}\frac{\Pi_\beta}{k_B\,n_\beta}\right),
\end{aligned}$$

with constants

$$
\begin{aligned}
\hat{c}_1(\alpha,\beta) &= \frac{m_\alpha\left(2a_\beta+\gamma_{\alpha\beta}+5\right)}{\left(\gamma_{\alpha\beta}+3\right)\left(m_\alpha+m_\beta\right)}\Big(m_\alpha\left(a_\alpha+1\right)+\frac{m_\beta}{2}\left(2a_\alpha+\gamma_{\alpha\beta}+5\right)\Big)>0,\\
\hat{c}_2(\alpha,\beta) &= \frac{\mathcal{C}_\alpha}{4\left(m_\alpha+m_\beta\right)}\Big(m_\alpha^2\left(2a_\beta+5\right)\left(2a_\alpha+\gamma_{\alpha\beta}+2\right)\\
&\quad+2m_\alpha m_\beta\left(2a_\beta+5\right)\left(2a_\alpha+\gamma_{\alpha\beta}+5\right)+2m_\beta^2\left(a_\beta+1\right)\left(2a_\alpha+\gamma_{\alpha\beta}+5\right)\Big)>0,\\
\hat{c}_3(\alpha,\beta) &= -\frac{1}{2\left(\gamma_{\alpha\beta}+3\right)\left(m_\alpha+m_\beta\right)}\Big(-3m_\alpha^2\left(2a_\beta+\gamma_{\alpha\beta}+5\right)+2m_\beta^2\gamma_{\alpha\beta}\left(a_\beta+1\right)\\
&\quad+m_\alpha m_\beta\left(\gamma_{\alpha\beta}\left(2a_\alpha+2\gamma_{\alpha\beta}+4a_\beta+15\right)+6a_\alpha+15\right)\Big)\\
\hat{c}_4(\alpha,\beta) &= -\frac{3}{2\left(a_\alpha+1\right)}\Big(-\hat{c}_2(\alpha,\beta)\\
&\quad+\frac{\left(2a_\alpha+5\right)m_\beta\,\mathcal{C}_\alpha}{4\left(m_\alpha+m_\beta\right)}\left(m_\alpha\left(2\left(a_\alpha+2a_\beta+6\right)+\gamma_{\alpha\beta}\right)+2\left(a_\beta+1\right)m_\beta\right)\\
&\quad-\frac{\left(a_\alpha+1\right)m_\alpha\,\mathcal{C}_\beta}{2\left(m_\alpha+m_\beta\right)}\left(m_\alpha\left(\gamma_{\alpha\beta}+2a_\beta+5\right)-\left(2a_\alpha+5\right)m_\beta\right)\Big).
\end{aligned}
$$

The final form (84) is obtained by denoting

$$
\begin{aligned}
\mathcal{E}_{\alpha\beta}^{T} &= \mathcal{K}_{\alpha\beta}\Big(\mathfrak{h}_1\left[\hat{c}_1(\alpha,\beta)+\hat{c}_1(\beta,\alpha)\right]+\mathfrak{h}_2\left[\hat{c}_2(\alpha,\beta)+\hat{c}_2(\beta,\alpha)\right]\Big),\\
\mathcal{E}_{\alpha\beta}^{\Pi} &= \mathcal{K}_{\alpha\beta}\Big(\mathfrak{h}_1\hat{c}_3(\alpha,\beta)+\mathfrak{h}_2\,\hat{c}_4(\alpha,\beta)\Big).
\end{aligned}
\tag{A31}
$$

References

1. De Groot, S.R.; Mazur, P. *Non-Equilibrium Thermodynamics*; North-Holland Publishing Company: Amsterdam, The Netherlands, 1962.
2. Giovangigli, V. *Multicomponent Flow Modeling*; Birkhäuser: Boston, MA, USA, 1999.
3. Nagnibeda, E.; Kustova, E. *Non-Equilibrium Reacting Gas Flows: Kinetic Theory of Transport and Relaxation Processes*; Springer: Berlin, Germany, 2009.
4. Müller, I.; Ruggeri, T. *Rational Extended Thermodynamics*; Springer: New York, NY, USA, 1998.
5. Truesdell, C. *Rational Thermodynamics*; Springer: New York, NY, USA, 1984.
6. Ruggeri, T.; Simić, S. On the hyperbolic system of a mixture of Eulerian fluids: a comparison between single-and multi-temperature models. *Math. Methods Appl. Sci.* **2007**, *30*, 827–849. [CrossRef]
7. Simić, S.; Pavić-Čolić, M.; Madjarević, D. Non-equilibrium mixtures of gases: Modelling and computation. *Riv. Mat. Della Univ. Parma* **2015**, *6*, 135–214.
8. Gouin, H.; Ruggeri, T. Identification of an average temperature and a dynamical pressure in a multi- temperature mixture of fluids. *Phys. Rev. E* **2008**, *78*, 016303. [CrossRef] [PubMed]
9. Ruggeri, T.; Simić, S. Average temperature and maxwellian iteration in multitemperature mixtures of fluids. *Phys. Rev. E* **2009**, *80*, 026317. [CrossRef] [PubMed]
10. Ruggeri, T.; Simić, S. Non-equilibrium diffusion temperatures in mixture of gases via Maxwellian iteration. *Ric. Mat.* **2017**, *66*, 293–312. [CrossRef]
11. Madjarević, D.; Simić, S. Shock structure in helium-argon mixture—A comparison of hyperbolic multi-temperature model with experiment. *EPL (Europhys. Lett.)* **2013**, *102*, 44002. [CrossRef]
12. Madjarević, D.; Ruggeri, T.; Simić, S. Shock structure and temperature overshoot in macroscopic multi-temperature model of mixtures. *Phys. Fluids* **2014**, *26*, 106102. [CrossRef]
13. Ruggeri, T.; Taniguchi, S. A complete classification of sub-shocks in the shock structure of a binary mixture of Eulerian gases with different degrees of freedom. *Phys. Fluids* **2022**, *34*, 066116. [CrossRef]
14. Torrilhon, M. Modeling Nonequilibrium Gas Flow Based on Moment Equations. *Annu. Rev. Fluid Mech.* **2016**, *48*, 429–458. [CrossRef]
15. Grad, H. On the kinetic theory of rarefied gases. *Commun. Pure Appl. Math.* **1949**, *2*, 331–407. [CrossRef]
16. Kogan, M.N. *Rarefied Gas Dynamics*; Plenum Press: New York, NY, USA, 1969.
17. Dreyer, W. Maximisation of the entropy in non-equilibrium. *J. Phys. A Math. Gen.* **1987**, *20*, 6505–6517. [CrossRef]
18. Levermore, C.D. Moment Closure Hierarchies for Kinetic Theories. *J. Stat. Phys.* **1996**, *83*, 1021–1065. [CrossRef]

19. Bisi, M.; Martalò, G.; Spiga, G. Multi-temperature Euler hydrodynamics for a reacting gas from a kinetic approach to rarefied mixtures with resonant collisions. *EPL (Europhys. Lett.)* **2011**, *95*, 55002. [CrossRef]
20. Ruggeri, T.; Sugiyama, M. *Rational Extended Thermodynamics Beyond the Monatomic Gas*; Springer: New York, NY, USA, 2015.
21. Ruggeri, T.; Sugiyama, M. *Classical and Relativistic Rational Extended Thermodynamics of Gases*; Springer Nature: Cham, Switzerland, 2021.
22. Bourgat, J.-F.; Desvillettes, L.; Le Tallec, P.; Perthame, B. Microreversible collisions for polyatomic gases. *Eur. J. Mech. B Fluids* **1994**, *13*, 237–254.
23. Desvillettes, L.; Monaco, R.; Salvarani, F. A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions. *Eur. J. Mech. B Fluids* **2005**, *24*, 219. [CrossRef]
24. Arima, T.; Taniguchi, S.; Ruggeri, T.; Sugiyama, M. Extended thermodynamics of dense gases. *Contin. Mech. Thermodyn.* **2012**, *24*, 271–292. [CrossRef]
25. Pavić, M.; Ruggeri, T.; Simić, S. Maximum entropy principle for rarefied polyatomic gases. *Phys. A* **2013**, *392*, 1302–1317. [CrossRef]
26. Pavić-Čolić, M.; Simić, S. Moment equations for polyatomic gases. *Acta Appl. Math.* **2014**, *132*, 469–482. [CrossRef]
27. Djordjić, V.; Pavić-Čolić, M.; Spasojević, N. Polytropic gas modelling at kinetic and macroscopic levels. *Kinet. Relat. Models* **2021**, *14*, 483–522. [CrossRef]
28. Pavić-Čolić, M.; Simić, S. Kinetic description of polyatomic gases with temperature-dependent specific heats. *Phys. Rev. Fluids* **2022**, *7*, 083401. [CrossRef]
29. Djordjić, V.; Pavić-Čolić, M.; Torrilhon, M. Consistent, Explicit and Accessible Boltzmann Collision Operator for Polyatomic Gases. *Phys. Rev. E* **2021**, *104*, 025309. [CrossRef] [PubMed]
30. Djordjić, V.; Oblapenko, G.; Pavić-Čolić, M.;Torrilhon, M. Boltzmann collision operator for polyatomic gases in agreement with experimental data and DSMC method. *Contin. Mech. Thermodyn.* **2022** . [CrossRef]
31. Arima, T.; Taniguchi, S.; Ruggeri, T.; Sugiyama, M. Extended thermodynamics of real gases with dynamic pressure: An extension of Meixner's theory. *Phys. Lett. A* **2012**, *376*, 2799–2803. [CrossRef]
32. Arima, T.; Ruggeri, T.; Sugiyama, M.; Taniguchi, S. Non-linear extended thermodynamics of real gases with 6 fields. *Int. J. Non Linear Mech.* **2015**, *72*, 6–15. [CrossRef]
33. Ruggeri, T. Non-linear maximum entropy principle for a polyatomic gas subject to the dynamic pressure. *Bull. Inst. Math. Acad. Sin.* **2016**, *11*, 1–22.
34. Pavić-Čolić, M.; Madjarević, D.; Simić, S. Polyatomic gases with dynamic pressure: Kinetic non-linear closure and the shock structure. *Int. J. Non Linear Mech.* **2017**, *92*, 160–175. [CrossRef]
35. Cramer, M.S. Numerical estimates for the bulk viscosity of ideal gases. *Phys. Fluids* **2012**, *24*, 066102. [CrossRef]
36. Kustova, E.; Mekhonoshina, M.; Kosareva, A. Relaxation processes in carbon dioxide. *Phys. Fluids* **2019**, *31*, 046104. [CrossRef]
37. Kosuge, S.; Aoki, K. Shock-wave structure for a polyatomic gas with large bulk viscosity. *Phys. Rev. Fluids* **2018**, *3*, 023401. [CrossRef]
38. Gamba, I.M.; Pavić-Čolić, M. On the Cauchy problem for Boltzmann equation modelling a polyatomic gas. *arXiv* **2022**, arXiv:2005.01017.
39. Alonso, R.; Gamba, I.M.; Pavić-Čolić, M. The Cauchy problem for Boltzmann systems modelling the mixing of monatomic and polyatomic gases. *Preprint* **2022** .
40. Pavić-Čolić, M. Multi-velocity and multi-temperature model of the mixture of polyatomic gases issuing from kinetic theory. *Physics Lett. A* **2019**, *383*, 2829–2835. [CrossRef]
41. Madjarević, D.; Pavić-Čolić, M.; Simić, S. Shock Structure and Relaxation in the Multi-Component Mixture of Euler Fluids. *Symmetry* **2021**, *13*, 955. [CrossRef]
42. Ruggeri, T. Galilean Invariance and Entropy Principle for Systems of Balance Laws. The Structure of the Extended Thermodynamics. *Continuum Mech. Thermodyn.* **1989**, *1*, 3–20. [CrossRef]
43. Liu, I.-S. Method of Lagrange multipliers for exploitation of the entropy principle. *Arch. Ration. Mech. Anal.* **1972**, *46*, 131–148. [CrossRef]
44. Boillat, G.; Ruggeri T. Hyperbolic principal subsystems: Entropy convexity and subcharacteristic conditions. *Arch. Ration. Mech. Anal.* **1997**, *137*, 305–320. [CrossRef]
45. Abramowitz, M.; Stegun, I.A. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*; National Bureau of Standards, U.S. Government Printing Office: Washington, DC, USA, 1964.