

Formal derivation of an isentropic two-phase flow model from the multispecies Boltzmann equation

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Starting from the multispecies Boltzmann equation for a gas mixture, we propose the formal derivation of the isentropic two-phase flow model introduced in E. Romenski, D. Drikakis, and E. Toro [J. Sci. Comput. **42**, 68 (2010)]. We examine the asymptotic limit as the Knudsen numbers approach zero, in a regime characterized by resonant intraspecies collisions, where interactions between particles of the same species dominate. This specific regime leads to a multivelocidity and multipressure hydrodynamic model, enabling the explicit computation of the coefficients for the two-phase macroscopic model. Our derivation also accounts for the inclusion of the evolution of the volume fraction, which is a key variable in many macroscopic multiphase models.

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I. INTRODUCTION

Multiphase flow models are widely used for the description of fluids with different physical or thermodynamic properties, usually separated by interfaces which are assumed to be diffuse. In these diffuse interface models, the fluids have different macroscopic properties but are allowed to mix across the interface zone. One of the first models of this type was introduced by Baer and Nunziato [1] and it is still the basis for the development of new strategies to describe compressible two-phase flows. After this pioneering work, many other models were proposed to approximate multiphase fluids, introducing some slight modifications to the original system regarding closure relations and relaxation parameters; see Refs. [2–6]. Their derivation is mainly based on phenomenological assumptions, which affect the validity of the model in more general situations. An alternative approach to the Baer-Nunziato model is the hyperbolic multiphase model introduced by Romenski, Drikakis and Toro [7,8], based on the theory of symmetric hyperbolic thermodynamically compatible systems [9]. Despite the fact that this model has been validated from a numerical point of view (see Ref. [10] for its approximation in all Mach number regimes and Ref. [11] for a complete analysis on the Riemann problem in the barotropic case), the derivation has an intrinsic

phenomenological nature and it contains some coefficients which cannot be explicitly determined. The purpose of the present paper is a formal derivation of macroscopic equations for multiphase flows from Boltzmann equations for mixtures of rarefied gases.

The behavior of rarefied gases is usually modeled through kinetic theory, in order to reproduce nonequilibrium phenomena. The seminal Boltzmann equation represents the cornerstone to describe the dynamics of a gas which is not in thermodynamical equilibrium, composed by a very large number of identical particles [12,13].

The necessity of studying systems involving gases composed of molecules of different types leads to kinetic models for mixtures. Indeed, realistic kinetic approximations of such situations can be performed only through multispecies models, in which interactions and exchanges between different components must be properly described. Although the mathematical properties of the Boltzmann equation for a single-species gas are well known, the analytical study of multispecies kinetic models is still not complete. Most of the literature concerns theory for Bhatnagar-Gross-Krook (BGK) models for gas mixtures [14–18]. To the best of our knowledge, the first derivation of the Boltzmann equation for binary gas mixtures is due to Chapman and Cowling [19]. The derivation of the expressions for transport coefficients has been performed in the work of Morse [20], within the framework of the Boltzmann equation. More recently, Briant and coauthors [21,22] have investigated the existence, uniqueness, positivity, and exponential trend to equilibrium for the linearized version of the full nonlinear Boltzmann equation in a perturbative isotropic $L_v^1 L_x^\infty$ setting, namely L^1 in velocity space and L^∞ in

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the physical space. A spectral gap for the linearized operator around global equilibrium has been proven in Ref. [22], then extended in Ref. [23] to the case of the linearized operator around nonequilibrium states and in Ref. [24], providing the explicit spectral gap for the linearized operator modeling reactive mixtures. In another recent paper, Gamba and Pavić-Čolić [25] have given an existence and uniqueness result for the spatially homogeneous multispecies Boltzmann equations with binary interactions in the Banach space represented by the L^1 space weighted polynomially in velocity. Properties of such solutions have been later analyzed in Ref. [26]. Further investigations on the mixing of monatomic and polyatomic gases can be found in Ref. [27].

The formal hydrodynamic limit for kinetic mixtures has been investigated for different regimes, both for the BGK model [28], for a mixed BGK-Boltzmann model [29,30] and for the Boltzmann model [31–36]. Let us mention also the work of Briant and Grec [37] on the rigorous derivation of the Fick cross-diffusion system from the multispecies Boltzmann equation.

All hydrodynamic limits of the Boltzmann equation correspond to situations where the frequency of collisions is rapidly increasing. This means that the collision mechanism governed by the collision operator holds on a timescale which is much smaller than the observation timescale and we have an almost instantaneous convergence of the distribution function to thermodynamic equilibrium. We refer to the book of Saint-Raymond for a complete review of hydrodynamic limits of the Boltzmann equation in the single-species framework [38]. In any case, the fluid limit provides a set of equations for the macroscopic fields, obtained as moments of the kinetic distribution function. This approach leads to a hierarchy of equations coupling lower-order moments to those of higher order, which could be truncated to obtain the desired order of approximation [28]. In a very recent paper [39] the author has derived a multivelocity and multitemperature macroscopic model without phase separation obtained within extended thermodynamics from Boltzmann-like equations, for mixtures of monatomic and polyatomic gases.

The aim of this paper is to propose a formal derivation of the model proposed by Romenski, Drikakis, and Toro [7] using kinetic theory. In particular, after a brief introduction to the multispecies Boltzmann equation, we discuss a hydrodynamic limit for this model in the regime of resonant intraspecies collisions [40], namely when the interactions between particles of the same species represent the fast process of the dynamics. This regime allows fast convergence towards local “equilibria”, in which each species reaches its own velocity, whereas interspecies interactions are characterized by a much slower process. The novelty of the work lies in the justification of the different scalings, in the introduction of the notion of “volume fraction” starting from the kinetic formulation and in the use of the full Boltzmann collision operator. Retrieving the volume fraction directly from the kinetic description ensures a physically consistent link between microscopic particle dynamics and the macroscopic two-phase behavior. Moreover, deriving a rigorous constitutive law from the microscopic dynamics at the interface of two gases, we are able to recover the original model introduced in Ref. [7] and to propose explicit expressions for the coefficients appearing in the macroscopic

model. A Prandtl-type scaling is introduced to handle the interface, enabling a detailed description of the thin interfacial layer and the recovery of stress-tensor continuity across it.

To the best of our knowledge, the Prandtl-type scaling used to derive the continuity of the stress tensor has never been applied to this type of problems and the volume fraction (characteristic of two-phase flows) has never been properly defined starting from kinetic theory.

II. THE MULTISPECIES BOLTZMANN EQUATION

The derivation of the multispecies Boltzmann equation is mostly formal, unlike that of the single-species case. Indeed, it is possible to consider some modeling assumptions, extending the microscopic dynamics of the single-species case to gas mixtures, in which different species are taken into account.

Let us consider a mixture of M species, each described by a distribution function $f_p = f_p(t, x, v)$, where the mass of a molecule of component p is denoted by m_p . Given $x \in \Omega \in \mathbb{R}^d$, $v \in \mathbb{R}^d$, the distribution functions f_p evolve according to the so-called multispecies Boltzmann equation, which, in absence of external forces, takes the following form [22]:

$$\begin{cases} \partial_t f_p + v \cdot \nabla_x f_p = Q_p(\mathbf{f}), & p = 1, \dots, M, \\ Q_p(\mathbf{f}) = \sum_{q=1}^M \frac{1}{\varepsilon_{pq}} Q^{pq}(f_p, f_q), \\ f_p(0, x, v) = f_{p,0}(x, v), \end{cases} \quad (2.1)$$

where $\mathbf{f} = (f_1, \dots, f_M)$. The parameter $\varepsilon_{pq} > 0$ denotes the relative *Knudsen number* associated with collisions between particles of species p and species q , that is the ratio between the mean free path of particles before each collision and the length scale of observation. Therefore, ε_{pq} governs the frequency of collisions for the species p : Taking a small Knudsen number corresponds to more frequent collisions. This particular scaling of the Boltzmann equation is usually known as *hyperbolic scaling*. In many physical situations, defining the Knudsen number ε_{pq} for each type of collision between species p and q allows for a more accurate representation of multispecies kinetic effects [33,41], especially in systems where interspecies interactions dominate over intraspecies dynamics. Indeed, the mean free path and collision frequency may vary significantly depending on the interacting species, as investigated in Sec. III B.

The time evolution of the distribution function due to particle collisions in the Boltzmann equation is given by a sum of *collision operators* Q^{pq} , referred to as self-collision operators (or *intraspecies* collision operators) if $p = q$ and cross-collision operators (or *interspecies* collision operators) if $p \neq q$. The microscopic dynamics is fundamental to understand the formulation of the Boltzmann equation and to derive an explicit formulation for the collision operator in (2.1). We need the following reasonable assumptions:

- (i) The particles interact via *binary* collisions. This means that collisions between three or more particles can be neglected.
- (ii) These binary collisions are localized in space and time.

- (iii) Collisions preserve mass for each species, total momentum, and total kinetic energy, namely for two particles of species p and q involved in the collision it holds,

$$\begin{cases} m_p v' + m_q v'_* = m_p v + m_q v_*, \\ m_p |v'|^2 + m_q |v'_*|^2 = m_p |v|^2 + m_q |v_*|^2. \end{cases}$$

We avoid any superscripts v^p in the notations and we simply refer to the precollisional velocities as (v, v_*) and to the postcollisional ones as (v', v'_*) .

In particular, the conservation of total momentum and total energy yields the following parametrizations for the postcollisional velocities (v', v'_*) in terms of the precollisional ones (v, v_*) :

- (1) The ω representation

$$\begin{aligned} v' &= v - \frac{2m_q}{m_p + m_q} ((v - v_*) \cdot \omega) \omega, \\ v'_* &= v_* + \frac{2m_p}{m_p + m_q} ((v - v_*) \cdot \omega) \omega, \end{aligned} \quad (2.2)$$

where $\omega \in \mathbb{S}^{d-1}$.

- (2) The σ representation

$$\begin{aligned} v' &= \frac{m_p v + m_q v_*}{m_p + m_q} + \frac{m_q}{m_p + m_q} |v - v_*| \sigma, \\ v'_* &= \frac{m_p v + m_q v_*}{m_p + m_q} - \frac{m_p}{m_p + m_q} |v - v_*| \sigma, \end{aligned} \quad (2.3)$$

where $\sigma \in \mathbb{S}^{d-1}$.

The σ representation is related to the ω -one through the following relation:

$$((v - v_*) \cdot \omega) \omega = \frac{1}{2} (v - v_* - |v - v_*| \sigma). \quad (2.4)$$

Defining $\mathcal{V}$ as the velocity of the center of mass of the particles p and q :

$$\mathcal{V} = \frac{m_p}{m_p + m_q} v + \frac{m_q}{m_p + m_q} v_*, \quad (2.5)$$

the laws of elastic collisions gives

$$v = \mathcal{V} + \frac{m_q}{m_p + m_q} (v - v_*) \quad v_* = \mathcal{V} - \frac{m_p}{m_p + m_q} (v - v_*). \quad (2.6)$$

and we can also rewrite the postcollisional velocities as

$$v' = \mathcal{V} + \frac{m_q}{m_p + m_q} (v' - v_*) \quad v'_* = \mathcal{V} - \frac{m_p}{m_p + m_q} (v' - v'_*). \quad (2.7)$$

Hence, the points v, v_*, v' , and v'_* belong to the plane defined by $\mathcal{V}$ and $\text{Span}(\sigma, v - v_*)$ and we have the geometric configuration in Fig. 1. The angle θ depends on σ according to the relation

$$\cos \theta := \frac{v - v_*}{|v - v_*|} \cdot \sigma. \quad (2.8)$$

Using the microscopic hypotheses (i), (ii), and (iii), it is possible to derive the explicit expression for the strong form

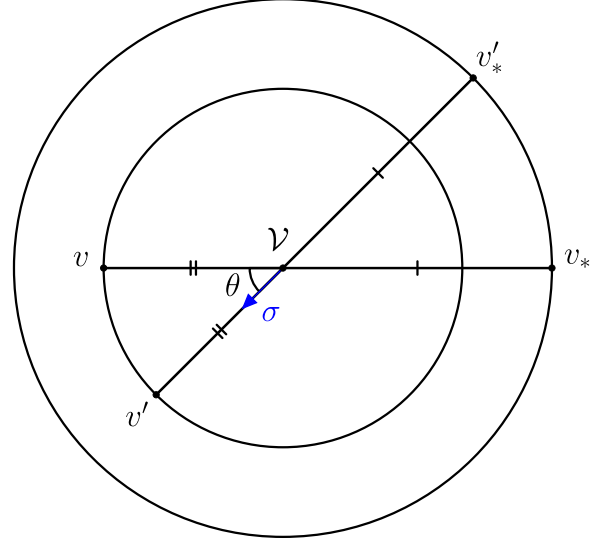


FIG. 1. Geometrical configuration of elastic collisions.

of the collision operators as

$$\begin{aligned} Q^{pq}(f_p, f_q) &= \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \mathbf{B}_{pq}(|v - v_*|, \theta) \\ &\quad \times [f_q(v'_*) f_p(v') - f_q(v_*) f_p(v)] d\Omega dv_*. \end{aligned} \quad (2.9)$$

The collision kernels $\mathbf{B}_{pq}$ are non-negative functions, which contain all the physical information about particles interactions, we refer to Refs. [12,13] for a detailed analysis on this subject.

In the following, we consider a collision kernel $\mathbf{B}_{pq}$ which depends only on $|v - v_*|$ and $\cos \theta$. For a general spherically symmetrical intermolecular potential $\Phi(r)$, the deflection angle θ is given by [19,42]:

$$\theta(|u|) = \pi - 2 \int_0^{W_1} \left[1 - W^2 - \frac{4\Phi(r)}{m|u|^2} \right]^{-1/2} dW, \quad (2.10)$$

where $W = d_p \cos(\theta/2)/r$, W_1 is the positive root of the term in the brackets, d_p is the molecular diameter, and r is the distance between two molecules. For the case of $(k-1)$ th inverse-power laws, namely for a potential of the form $\Phi(r) \propto 1/(k-1)r^{k-1}$, the relevant simplification is that $\mathbf{B}_{pq}(|v - v_*|, \theta)$ becomes the product of a function of θ alone by a fractional power of $|v - v_*|$. Thus, in the case of inverse-power-law potentials, it is possible to rewrite the collision kernel as [42]

$$\mathbf{B}_{pq}(|v - v_*|, \theta) = b_{pq}(\theta) |v - v_*|^\gamma, \quad \gamma = \frac{k - (2d - 1)}{k - 1}, \quad (2.11)$$

where $b_{pq}(\theta)$ is a nonelementary function of θ . In particular, in $d = 3$ dimensions of space, we obtain $\gamma = (k - 5)/(k - 1)$. Thus, the choice $k = 5$ corresponds to the particular case in which the collision kernel does not depend on the relative velocity but only on the deviation angle. Such particles are called Maxwellian molecules and $\mathbf{B}_{pq}(|v - v_*|, \theta) = b_{pq}(\cos \theta)$. The pseudo-Maxwellian case is given by a constant value of $b_\gamma(\cos \theta)$. For numeri-

cal purpose a widely adopted model is the variable hard sphere model introduced by Bird [42], corresponding to the choice $b_{pq}(\cos \theta) = C_\gamma$, where $C_\gamma > 0$. The case $\gamma = 0$ is the aforementioned pseudo-Maxwellian molecules case, whereas $\gamma = 1$ gives the hard-spheres molecules case.

The hypothesis of constant γ for different species could be weakened, for instance, by considering a collision kernel (2.11) with different γ_p according to the species p , as done in Ref. [27], but it does not affect the main conclusions of this work.

A. Weak form

In this section we investigate the weak form of the multispecies Boltzmann equation, following the clear derivation presented in Ref. [36] (see also Ref. [12] for the single-species case). The operators Q^{pp} are the classical Boltzmann collision operators. Starting from the definition of velocities obtained in (2.3) and using the microscopic hypotheses, we derive the *weak form* in the σ representation, considering a C^∞ test function $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$. We assume that the cross section $\mathbf{B}_{pq}$ satisfies the microreversibility assumption $\mathbf{B}_{pq}(v, v_*, \sigma) = \mathbf{B}_{pq}(v_*, v, \sigma)$. We obtain

$$\begin{aligned} & \int_{\mathbb{R}^d} Q^{pp}(f_p, f_p)(v) \psi(v) dv \\ &= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} f_{p*} f_p (\psi' + \psi'_* - \psi - \psi_*) \\ & \quad \times \mathbf{B}_{pp}(|v - v_*|, \cos \theta) d\sigma dv dv_*, \end{aligned} \quad (2.12)$$

where we have introduced the shorthands $f'_p = f_p(v')$, $f_{p*} = f_p(v_*)$, $f'_{p*} = f_p(v'_*)$, $\psi' = \psi(v')$, $\psi_* = \psi(v_*)$, and $\psi'_* = \psi(v'_*)$.

In an analogous way, it is possible to characterize the bispecies collision operators. Therefore, considering the definition (2.3) with $p \neq q$, in the same way of the monospecies framework, we obtain the following formulation of Q^{pq} in the σ representation:

$$\begin{aligned} & \int_{\mathbb{R}^d} Q^{pq}(f_p, f_q)(v) \psi(v) dv \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} f_p f_{q*} (\psi' - \psi) \mathbf{B}_{pq}(|v - v_*|, \cos \theta) d\sigma dv dv_*. \end{aligned} \quad (2.13)$$

In addition, if we consider both the bispecies collision operators, then we can give the following characterization:

$$\begin{aligned} & \int_{\mathbb{R}^d} Q^{pq}(f_p, f_q)(v) \psi(v) dv + \int_{\mathbb{R}^d} Q^{qp}(f_q, f_p)(v) \phi(v) dv \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} f_p f_{q*} (\psi' + \phi'_* - \psi - \phi_*) \\ & \quad \times \mathbf{B}_{pq}(|v - v_*|, \cos \theta) d\sigma dv dv_*, \end{aligned} \quad (2.14)$$

for any C^∞ test functions $\psi, \phi : \mathbb{R}^d \rightarrow \mathbb{R}$.

Using the weak form, one can easily observe that the conservation properties of the Boltzmann equation are extended to the multispecies cases. The mass of each species is

conserved, since

$$\int_{\mathbb{R}^d} Q_p(f, g)(v) dv = 0, \quad (2.15)$$

for any functions $f(v)$ and $g(v)$, namely the constant function $v \mapsto 1$ is a collisional invariant for this operator. On the other hand, the functions v and $|v|^2$ are not collision invariants, but it holds that

$$\int_{\mathbb{R}^d} m_p v Q^{pq}(f, g)(v) dv = - \int_{\mathbb{R}^d} m_q v Q^{qp}(g, f)(v) dv, \quad (2.16)$$

and

$$\int_{\mathbb{R}^d} m_p |v|^2 Q^{pq}(f, g)(v) dv = - \int_{\mathbb{R}^d} m_q |v|^2 Q^{qp}(g, f)(v) dv. \quad (2.17)$$

In particular, the choice of $\psi(v) = m_i v$ and $\phi(v) = m_j v$ in (2.14) leads to the conservation of the total momentum, whereas $\psi(v) = m_i |v|^2$ and $\phi(v) = m_j |v|^2$ leads to the conservation of the total kinetic energy of the mixture.

B. Macroscopic quantities

Let us define the macroscopic fields for each species as suitable moments of the distribution functions f_p . In particular, the number density n_p , the mass density ρ_p , the average macroscopic velocity $\bar{u}_p$, the partial pressure P_p , and the temperature $\bar{T}_p$ for each species are computed as

$$\begin{aligned} n_p &= \int_{\mathbb{R}^d} f_p(v) dv, \quad \rho_p \bar{u}_p = \int_{\mathbb{R}^d} m_p v f_p dv, \\ \bar{T}_p &= \frac{m_p}{d n_p} \int_{\mathbb{R}^d} |v - \bar{u}_p|^2 f_p dv, \end{aligned} \quad (2.18)$$

with $\rho_p = m_p n_p$ and $P_p = n_p \bar{T}_p$. We can also define the total moments for the mixture, given by

$$\begin{aligned} n &= \sum_p n_p, \quad \rho = \sum_p \rho_p, \quad \rho \bar{u} = \sum_p \rho \bar{u}_p, \\ P &= \sum_p P_p, \quad \bar{T} = \sum_p \frac{m_p}{d n_p} \int_{\mathbb{R}^d} |v - \bar{u}|^2 f_p dv. \end{aligned} \quad (2.19)$$

All these quantities are valid for situations in which the two species are not well separated. When we deal with gases in which species are segregated, intraspecies collisions become more frequent and different regimes must be taken into account. For this purpose, we introduce a new quantity α_p , describing the volume fraction occupied by the species p . Heuristically, let us consider a control volume V and let $\chi_p(x, t)$ be the probability of finding a particle of the species p in (x, t) . Then the volume fraction $\alpha_p(x, t)$ occupied by the phase p is defined as

$$\alpha_p(x, t) = \frac{1}{|V|} \int_V \chi_p(x, t) dV. \quad (2.20)$$

In this setting, $\sum_p \alpha_p = 1$ and the situation is depicted in Fig. 2 for a mixture of two species. The volume fraction α_p represents the key factor for the hydrodynamic limit performed in Sec. III B. By introducing the volume fraction within the kinetic framework, the macroscopic two-phase

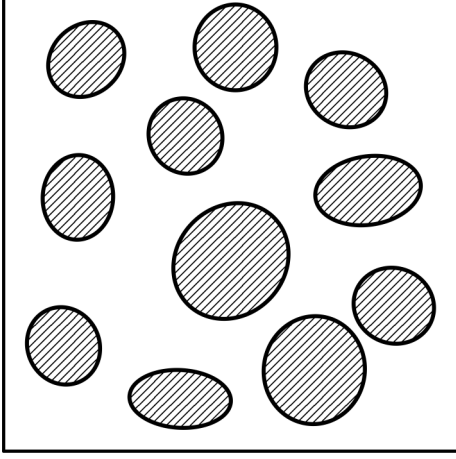


FIG. 2. Diffuse interface gases in a control volume.

model naturally inherits physical consistency from the microscopic particle dynamics. Moreover, we observe that if the two gases are identical, then both the Boltzmann formulation and the macroscopic description reduce to the single-gas case.

Remark 2.1. The role of the volume fraction for each species is fundamental for models of separated gases [1,7]. Indeed, in the passage to the macroscopic level, the system could be described using volume fractions that smoothly vary from one region to the other in the space scale of the control volume V .

C. Entropy dissipation

The large-time behavior of the multispecies Boltzmann equation (2.1) is here briefly described. In this subsection we restrict our analysis to the case of a bispecies mixture for the sake of simplicity, but it can be easily extended to the case of M -species mixtures. In particular, we will consider the space homogeneous setting,

$$\begin{cases} \partial_t f_1 = Q^{11}(f_1, f_1) + Q^{12}(f_1, f_2), \\ \partial_t f_2 = Q^{21}(f_2, f_1) + Q^{22}(f_2, f_2). \end{cases} \quad (2.21)$$

Definition 2.1 (multispecies entropy). Let (f_1, f_2) be a solution to the homogeneous Boltzmann equation (2.21). The multispecies entropy is described by the so-called Boltzmann's H -functional,

$$H = \int_{\mathbb{R}^d} f_1 \ln f_1(v) dv + \int_{\mathbb{R}^d} f_2 \ln f_2(v) dv. \quad (2.22)$$

Remark 2.2. This definition can be easily extended to the case of $M \geq 2$ species by defining

$$H = \sum_{i=1}^M \int_{\mathbb{R}^d} f_p \ln f_p(v) dv. \quad (2.23)$$

Let us now recall the following result on entropy dissipation, proven in Ref. [43], here explicitly detailed for a nonreactive mixture of two species.

Proposition 2.1. Let us assume strictly positive collision kernels $\mathbf{B}_{pq}$ and let us consider a positive solution (f_1, f_2) to (2.1). Then, the entropy is dissipated, namely

$$\frac{dH}{dt} \leq 0. \quad (2.24)$$

Moreover, we have $\frac{dH}{dt} = 0$ if and only if the equilibrium (f_1, f_2) is given by a pair of global Maxwellian distributions $(\mathcal{M}_1, \mathcal{M}_2)$ with common average velocity $\bar{u}$ and temperature $\bar{T}$,

$$\begin{aligned} \mathcal{M}_p^{n_p, \bar{u}, \bar{T}}(t, x, v) &= n_p \left(\frac{m_p}{2\pi\bar{T}} \right)^{\frac{d}{2}} \exp \left(-\frac{m_p}{2\bar{T}} |\bar{u} - v|^2 \right), \\ p &= 1, 2. \end{aligned} \quad (2.25)$$

Sketch of the proof. Let us consider the expression

$$\begin{aligned} \frac{dH}{dt} &= \int_{\mathbb{R}^d} Q^{11}(f_1, f_1) \ln f_1(v) dv \\ &\quad + \int_{\mathbb{R}^d} Q^{12}(f_1, f_2) \ln f_1(v) dv \\ &\quad + \int_{\mathbb{R}^d} Q^{21}(f_2, f_1) \ln f_2(v) dv \\ &\quad + \int_{\mathbb{R}^d} Q^{22}(f_2, f_2) \ln f_2(v) dv. \end{aligned} \quad (2.26)$$

We consider the weak formulation of the collision operators (2.12)–(2.14) with $\phi = \ln f_1$ and $\psi = \ln f_2$:

$$\begin{aligned} \frac{dH}{dt} &= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} f_{1*} f_1 \ln \left(\frac{f'_1 f'_{1*}}{f_1 f_{1*}} \right) \mathbf{B}_{11} d\sigma dv dv_* - \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} [f'_1 f'_{2*} - f_1 f_{2*}] \ln \left(\frac{f'_1 f'_{2*}}{f_1 f_{2*}} \right) \mathbf{B}_{12} d\sigma dv dv_* \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} f_{2*} f_2 \ln \left(\frac{f'_2 f'_{2*}}{f_2 f_{2*}} \right) \mathbf{B}_{22} d\sigma dv dv_* \\ &= \frac{1}{2} \sum_{p,q \in \{1,2\}} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} f_{p*} f_q \left[\ln \left(\frac{f'_p f'_{q*}}{f_p f_{q*}} \right) - \frac{f'_p f'_{q*}}{f_p f_{q*}} + 1 \right] \mathbf{B}_{pq} d\sigma dv dv_* \\ &\quad + \frac{1}{2} \sum_{p,q \in \{1,2\}} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} (f'_{q*} f'_p - f_{q*} f_p) \mathbf{B}_{pq} d\sigma dv dv_* \leq 0. \end{aligned}$$

Indeed, since we are assuming strictly positive cross sections, $\ln x - x + 1 \leq 0$ and the collisional transformation $(v, v_*) \rightarrow (v', v'_*)$ is an involution, all terms on the right-hand side of the equation above are nonpositive and this proves the entropy dissipation.

To prove the second part, we first observe that, since we are considering a sum of nonpositive contributions, $\frac{dH}{dt} = 0$ implies that all these terms must be zero. The terms corresponding to intraspecies collisions (namely depending only on f_p) vanish if there exist $n_p \geq 0$, $\bar{u}_p \in \mathbb{R}^d$, and $\bar{T}_p > 0$ such that

$$f_p(v) = n_p \left(\frac{m_p}{2\pi\bar{T}_p} \right)^{\frac{d}{2}} \exp \left(-\frac{m_p}{2\bar{T}_p} |\bar{u}_p - v|^2 \right), \quad p = 1, 2. \quad (2.27)$$

To conclude the proof, in Ref. [43] the authors prove that $\bar{u}_1 = \bar{u}_2 = \bar{u}$ and $\bar{T}_1 = \bar{T}_2 = \bar{T}$.

Remark 2.3. Let us underline that the *local* Maxwellians $\mathcal{M}_p(t, x, v)$ defined in (2.27) are maximum of the Boltzmann entropy in the monospecies setting, but they are not local equilibria for the gas mixture. Nevertheless, they play a fundamental role in the derivation of hydrodynamic limits for different regimes.

Let us consider the inhomogeneous system with a hyperbolic scaling ε , under the assumption that the relaxation velocity is the same for each collision operator, namely

$$\begin{cases} \partial_t f_1 + v \cdot \nabla_x f_1 = \frac{1}{\varepsilon} Q^{11}(f_1, f_1) + \frac{1}{\varepsilon} Q^{12}(f_1, f_2), \\ \partial_t f_2 + v \cdot \nabla_x f_2 = \frac{1}{\varepsilon} Q^{21}(f_2, f_1) + \frac{1}{\varepsilon} Q^{22}(f_2, f_2). \end{cases} \quad (2.28)$$

In this framework, the equilibrium (f_1, f_2) is reached in the limit $\varepsilon \rightarrow 0$ and the distribution functions converge towards Maxwellian functions with common average velocity and temperature, as shown in Proposition 2.1.

In mixtures of gases with disparate masses the exchange of momentum between particles of the same species is usually a faster process and the relaxation velocity is not the same for each collision operator. This regime is physically realistic, e.g., for mixtures of heavy and light gases, usually referred to as ε mixtures, as described in Refs. [28,40]. For the sake of completeness, we also mention the work of Degond and Lucquin-Desreux [41], in which electron-ion mixtures are investigated.

In our regime, the inhomogeneous system is scaled as follows:

$$\begin{cases} \partial_t f_1 + v \cdot \nabla_x f_1 = \frac{1}{\varepsilon} Q^{11}(f_1, f_1) + \frac{1}{\kappa} Q^{12}(f_1, f_2), \\ \partial_t f_2 + v \cdot \nabla_x f_2 = \frac{1}{\kappa} Q^{21}(f_2, f_1) + \frac{1}{\varepsilon} Q^{22}(f_2, f_2), \end{cases} \quad (2.29)$$

where $\varepsilon > 0$ and $\kappa > 0$ may not have the same order of magnitude. Despite the minimum of the entropy (the global equilibrium) is still a pair of global Maxwellian $(\mathcal{M}_1, \mathcal{M}_2)$, the dynamics involves processes at two different timescales and the convergence no longer occurs on the same timescale. Let us assume that the two species are segregated, as in Fig. 2. For the sake of illustration, we can think of a setting in which droplets (or bubbles) of light gas are separated by a heavy gas. The separation between the two species leads to a configuration in which interspecies collisions can occur only along the separation layers (*interface*). On the contrary, intraspecies

collisions can occur inside the volume (in Fig. 2, dashed volumes for one species and white for the other species). This corresponds to the regime $\kappa = \mathcal{O}(L/T)$, where L and T are the respective characteristic length and timescales, and $\varepsilon \ll \kappa$, in which intraspecies collisions are much more frequent than interspecies ones. In this case, for $\varepsilon \rightarrow 0$, each distribution function f_p converges towards the local Maxwellian (2.27) with local average velocity $\bar{u}_p$ and local temperature $\bar{T}_p$, before reaching a global equilibrium. The process which leads to common average velocities and common temperatures is much slower and we assume it can be disregarded for finite times.

III. HYDRODYNAMIC LIMIT FOR MULTISPECIES BOLTZMANN EQUATION

A. The single-velocity case

In this section we describe the formal derivation of the Euler equations from the multispecies Boltzmann equation, under the assumption that the Knudsen number is approximately the same for all species. In the limit of small Knudsen numbers, that is $\varepsilon \rightarrow 0$, the frequency of collisions increases to infinity and the solution can be completely described by its local hydrodynamic fields. To do so, we recall the multispecies Boltzmann equation rescaled according to the hyperbolic scaling, where all the collision operators scale with the same rate,

$$\partial_t f_p + v \cdot \nabla_x f_p = \frac{1}{\varepsilon} Q_p(\mathbf{f}) \quad p = 1, \dots, M, \quad (3.1)$$

and we apply the Chapman-Enskog expansion as in Ref. [28]. Formally, we can consider an expansion of the distribution functions in term of ε as

$$f_p = f_p^0 + \varepsilon f_p^1 + \mathcal{O}(\varepsilon^2), \quad (3.2)$$

obtaining expansions also for the other quantities of interest. In particular the number densities n_p , mass velocities $\bar{u}_p$, and temperatures $\bar{T}_p$ can be expanded as

$$\begin{aligned} n_p &= n_p^0 + \varepsilon n_p^1 + \mathcal{O}(\varepsilon^2), & \bar{u}_p &= \bar{u}_p^0 + \varepsilon \bar{u}_p^1 + \mathcal{O}(\varepsilon^2), \\ \bar{T}_p &= \bar{T}_p^0 + \varepsilon \bar{T}_p^1 + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (3.3)$$

Let us consider the weak form of the Boltzmann equation truncated at the zeroth order of expansion

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\mathbb{R}^d} \varphi(v) (f_p^0 + \varepsilon f_p^1) dv + \nabla_x \cdot \int_{\mathbb{R}^d} \varphi(v) v (f_p^0 + \varepsilon f_p^1) dv \\ = \frac{1}{\varepsilon} \sum_{q=1}^N \int_{\mathbb{R}^d} \varphi(v) Q^{pq}(f_p^0 + \varepsilon f_p^1, f_q^0 + \varepsilon f_q^1) dv, \end{aligned} \quad (3.4)$$

where $\varphi(v)$ is a $\mathcal{C}^\infty$ test function.

Remark 3.1. In the Chapman-Enskog expansion, f_p^1 designates a quantity that depends smoothly on the macroscopic quantities and any finite number of its derivatives with respect to the (x, v) variables (but not on time). In particular, f_p^1 satisfies

$$\int_{\mathbb{R}^d} f_p^1 \left(\frac{1}{\frac{1}{2}|v|^2} \right) dv = 0. \quad (3.5)$$

The limit for $\varepsilon \rightarrow 0$ in (3.1) implies naturally a vanishing leading-order collision operator, and thus f_i^0 are the Boltzmann equilibria (2.25). The 0th-order term of Eq. (3.4) provides the multispecies (or multicomponent) Euler equations for macroscopic quantities and the first-order correction corresponds to the multispecies (or multicomponent) Navier-Stokes system [44]. In other words, we can claim that formally the solution to the multispecies Euler equations and the solution to the multispecies Navier-Stokes equations are close to the moments of the solution f to the multispecies Boltzmann equation respectively at order $\mathcal{O}(\varepsilon)$ and $\mathcal{O}(\varepsilon^2)$.

The multispecies Euler system can be directly recovered with a different approach, considering the collision invariants as test functions in the weak formulation

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\mathbb{R}^d} \varphi(v) f_p dv + \nabla_x \cdot \int_{\mathbb{R}^d} \varphi(v) v f_p dv \\ = \sum_{q=1}^N \int_{\mathbb{R}^d} \varphi(v) Q^{pq}(f_p, f_q) dv. \end{aligned}$$

Let us consider $\varphi(v) \equiv 1$. Since it corresponds to a collision invariant of the Boltzmann operator, the right-hand side vanishes and it leads to the equation

$$\frac{\partial n_p}{\partial t} + \nabla_x \cdot (n_p \bar{u}) = 0, \quad p = 1, \dots, M, \quad (3.6)$$

where we have used $\bar{u}_p = \bar{u}$ for all p . Multiplying each equation for the respective mass m_p we obtain

$$\frac{\partial \rho_p}{\partial t} + \nabla_x \cdot (\rho_p \bar{u}) = 0, \quad p = 1, \dots, M. \quad (3.7)$$

Finally, summing over the index p , the continuity equation for the total density holds

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \bar{u}) = 0. \quad (3.8)$$

Now consider $\varphi(v) = m_p v$ and sum over the index p in order to obtain

$$\frac{\partial}{\partial t} (\rho \bar{u}) + \nabla_x \cdot \left[\sum_{p=0}^P (\rho_p \bar{u} \otimes \bar{u} + n_p \bar{T}) \right] = 0, \quad (3.9)$$

where the single-species temperature $\bar{T}_p = \bar{T}$. Let us consider $\varphi(v) = m_p |v|^2$ and sum again over the index p . Thus, we obtain

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\bar{u}|^2 + \frac{d}{2} n \bar{T} \right) + \nabla_x \cdot \left[\left(\frac{1}{2} \rho |\bar{u}|^2 + \frac{d+2}{2} n \bar{T} \right) \bar{u} \right] = 0. \quad (3.10)$$

Thus, in the limit $\varepsilon \rightarrow 0$, we have formally obtained the so-called multispecies Euler limit:

$$\begin{cases} \frac{\partial \rho_p}{\partial t} + \nabla_x \cdot (\rho_p \bar{u}) = 0, & p = 1, \dots, M, \\ \frac{\partial}{\partial t} (\rho \bar{u}) + \nabla_x \cdot \left[\sum_{p=1}^N \rho_p (\bar{u} \otimes \bar{u} + n_p \bar{T}) \right] = 0, \\ \frac{\partial}{\partial t} \left(\frac{1}{2} \rho |\bar{u}|^2 + \frac{d}{2} n \bar{T} \right) + \nabla_x \cdot \left[\left(\frac{1}{2} \rho |\bar{u}|^2 + \frac{d+2}{2} n \bar{T} \right) \bar{u} \right] = 0, \end{cases} \quad (3.11)$$

with a single velocity and a single temperature for the whole mixture.

B. The multivelocity case

Now, we are interested in describing the formal hydrodynamic limit in a different regime, in order to recover the isentropic two-phase flow model proposed in Ref. [7], which in the one-dimensional case reads as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho \bar{u}) = 0, \quad (3.12a)$$

$$\frac{\partial}{\partial t} (\alpha_1 \rho) + \frac{\partial}{\partial x} (\alpha_1 \rho \bar{u}) = -\frac{1}{\tau} (P_2 - P_1), \quad (3.12b)$$

$$\frac{\partial}{\partial t} (\alpha_1 \rho_1) + \frac{\partial}{\partial x} (\alpha_1 \rho_1 \bar{u}_1) = 0, \quad (3.12c)$$

$$\frac{\partial}{\partial t} (\rho \bar{u}) + \frac{\partial}{\partial x} (\alpha_1 \rho_1 \bar{u}_1^2 + \alpha_1 P_1 + \alpha_2 \rho_2 \bar{u}_2^2 + \alpha_2 P_2) = 0, \quad (3.12d)$$

$$\frac{\partial}{\partial t} (\bar{u}_1 - \bar{u}_2) + \frac{\partial}{\partial x} \left(\frac{1}{2} \bar{u}_1^2 + h_1 - \frac{1}{2} \bar{u}_2^2 - h_2 \right) = -\zeta (\bar{u}_1 - \bar{u}_2), \quad (3.12e)$$

where $\alpha_p \in (0, 1)$ is the volume fraction defined in (2.20), τ and ζ are opportune constants, and the partial pressures P_p will be described later. In this framework, the total density ρ is defined as

$$\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2, \quad (3.13)$$

and the mixture velocity $\bar{u}$ as

$$\bar{u} = \kappa_1 \bar{u}_1 + \kappa_2 \bar{u}_2, \quad \kappa_p = \frac{\alpha_p \rho_p}{\rho}. \quad (3.14)$$

Compared to the model of two-phase mixtures proposed by Baer and Nunziato [1], the main advantage of this alternative model is the possibility to write the equations in a conservative form.

Equations (3.12a) and (3.12c) describe the conservation of the total mass and the partial mass, respectively. Equation (3.12b) consists of the balance of the evolution of the volume fraction with respect to a pressure relaxation term. Further, Equation (3.12d) gives the conservation of the total momentum $\rho \bar{u}$ and Equation (3.12e) the balance of the relative velocity $\bar{u}_1 - \bar{u}_2$ with respect to a friction term.

Since the system (3.12a)–(3.12e) is isentropic, we set $P_p = P(\rho_p) = c \rho_p^\gamma$. This closure law for the pressure terms implies

that an equation for the second moment is not required, differently from (3.11).

To obtain the hyperbolic two-phase flow model as a limit system from a kinetic model, we take into account the case of a gas mixture as in Fig. 2. We recall that in this setting, self-collisions are much more frequent than collisions among particles of different species, namely $\kappa = 1$ and $\varepsilon \ll 1$ in (2.29), as described in Sec. II B. For this purpose, we then consider the following rescaling of the multispecies Boltzmann equation

$$\begin{cases} \partial_t f_p + v \cdot \nabla_x f_p = \frac{1}{\varepsilon} Q^{pp}(f_p, f_p) + \sum_{\substack{q=1 \\ q \neq p}}^M Q^{pq}(f_p, f_q), \\ f_p(0, x, v) = f_{p,0}(x, v). \end{cases} \quad (3.15)$$

The weak form of the Boltzmann equation in this scaling becomes

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\mathbb{R}^d} \varphi(v) f_p dv + \nabla_x \cdot \int_{\mathbb{R}^d} \varphi(v) v f_p dv \\ = \frac{1}{\varepsilon} \int_{\mathbb{R}^d} \varphi(v) Q^{pp}(f_p, f_p) dv \\ + \sum_{\substack{q=1 \\ q \neq p}}^M \int_{\mathbb{R}^d} \varphi(v) Q^{pq}(f_p, f_q) dv. \end{aligned} \quad (3.16)$$

Next, we average the weak form over the control volume V :

$$\begin{aligned} \int_V \chi_p \frac{\partial}{\partial t} \int_{\mathbb{R}^d} \varphi(v) f_p dv dV + \int_V \chi_p \nabla_x \cdot \int_{\mathbb{R}^d} \varphi(v) v f_p dv dV \\ = \frac{1}{\varepsilon} \int_V \chi_p \int_{\mathbb{R}^d} \varphi(v) Q^{pp}(f_p, f_p) dv dV \\ + \sum_{\substack{q=1 \\ q \neq p}}^M \int_V \chi_p \int_{\mathbb{R}^d} \varphi(v) Q^{pq}(f_p, f_q) dv dV, \end{aligned}$$

where χ_p is the probability to find a particle of species p in (x, t) . Each χ_p is associated to the corresponding volume fraction α_p , as introduced in (2.20). Averaging procedure is widely used in the derivation of multiphase models from the corresponding single-phase formulations (e.g., from multi-component Euler systems), see for instance Refs. [45,46]. In this work, the spatial averaging procedure is instead directly applied to the kinetic equation, following the same rules presented in Ref. [45]. Indeed, the averaging procedure over a control volume V commutes with time and space derivatives, and the following calculation rules hold for any function g :

(1) Gauss rule:

$$\int_V \chi_p \nabla_x g dV = \int_V \nabla_x (\chi_p g) dV - \int_V g_{\text{interface}} \nabla_x \chi_p dV,$$

(2) Leibniz rule:

$$\int_V \chi_p \partial_t g dV = \int_V \partial_t (\chi_p g) dV - \int_V g_{\text{interface}} \partial_t \chi_p dV,$$

where $g_{\text{interface}}$ is the value of g at ∂V . The boundary ∂V of the domain includes both the external physical boundary and all interfaces separating the phases, where state variables may exhibit discontinuities. Let us then define macroscopic fields

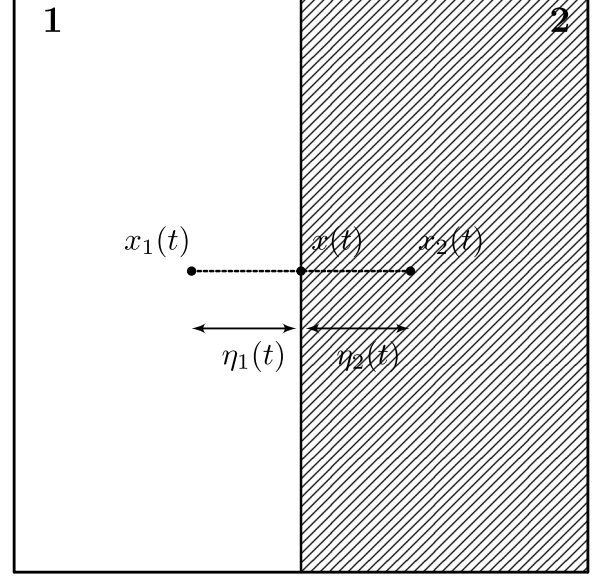


FIG. 3. Interface between two different species.

as moments of the distribution functions averaged over a unit control volume V (avoiding the scaling factor $|V|^{-1}$ for the sake of simplicity) according to the quantity χ_p , namely

$$\begin{aligned} \int_V \int_{\mathbb{R}^d} \chi_p m_p f_p(v) dv dV &= \alpha_p \rho_p, \\ \int_V \int_{\mathbb{R}^d} \chi_p m_p v f_p(v) dv dV &= \alpha_p \rho_p \bar{u}_p, \end{aligned} \quad (3.17)$$

where we recall that α_p stands for the volume fraction. This choice allows us to give a kinetic interpretation of the macroscopic quantities involved in (3.12a)–(3.12e). The probability χ_p evolves according to the equation

$$\partial_t \chi_p + \bar{u}_{\text{interface}} \cdot \nabla_x \chi_p = 0, \quad (3.18)$$

where $\bar{u}_{\text{interface}}$ is the interface velocity between the two phases.

Remark 3.2. The spatial average procedure is fundamental to obtain equations for different phases, describing “nonlocal” processes which happen at the scale of the control volume.

In order to derive the equation for the fraction α_1 , we have to determine an expression for the transfer of volume in the dynamics. We will show that the volume transfer is caused by the difference in pressures between the two gases, which in the literature is usually assumed as a phenomenological hypothesis [1,3,5]. Let us consider a zoom of the setting of Fig. 2 on the thin layer which separates the volume occupied by one species from the volume occupied by the other, as shown in Fig. 3. We now focus on the displacement of the interface separating the two species. Following the idea of Bresch, Burtea, and Lagoutière [47], at this scale the volume fraction variation can be reinterpreted as a one-dimensional shift orthogonal to the separating interface. Denoting with $x(t)$ the average distance of particles from the interface of separation between the two species, let us consider $\eta_1(t) := x_1(t) - x(t)$ and $\eta_2(t) := x(t) - x_2(t)$, where x_1 and x_2 are the

local centers of mass of the species 1 and 2, respectively. We indeed perform a spatial average over a thin layer which is much smaller than V , so we refer to the “centers of mass” of the molecules within this tiny volume.

Assuming that $\eta_p \ll \text{diameter}(V)$, let us define

$$\alpha_1(t) = \frac{\eta_1(t)}{\eta_1(t) + \eta_2(t)}. \quad (3.19)$$

Let us introduce the material derivative as

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + \bar{u} \cdot \nabla_x, \quad (3.20)$$

where we recall that $\bar{u}$ is the mixture velocity. Since we are considering segregated gases, the mixture velocity satisfies $\bar{u} = \bar{u}_p$ in the region occupied only by species p .

In the reference frame of the interface, the material derivative of the volume fraction α_1 is given by

$$\frac{D}{Dt} \alpha_1(t) = \frac{D_t \eta_1 (\eta_1 + \eta_2) - \eta_1 (D_t \eta_1 + D_t \eta_2)}{(\eta_1 + \eta_2)^2}, \quad (3.21)$$

where we have omitted the explicit dependence of η_p on time. As we considered a small shift with respect to the interface, we have

$$D_t \eta_p(t) = \bar{u}_p(t, x_p(t)) - \bar{u}(t, x(t)). \quad (3.22)$$

Therefore, the expression of the derivative of the volume fraction becomes

$$\begin{aligned} \frac{D}{Dt} \alpha_1(t) &= \frac{(\bar{u}_1(t) - \bar{u}(t))(\eta_1 + \eta_2) - \eta_1(\bar{u}_1(t) - \bar{u}_2(t))}{(\eta_1 + \eta_2)^2} \\ &= \frac{\eta_1(\bar{u}_2(t) - \bar{u}(t)) + \eta_2(\bar{u}_1(t) - \bar{u}(t))}{(\eta_1 + \eta_2)^2}. \end{aligned} \quad (3.23)$$

Let us assume that across the diffuse interface there is a “boundary layer” really separating the two gases, which provides the existence of a continuous stress tensor at the interface: Namely, given a coefficient λ representing the kinematic viscosity, the quantity

$$P(t, x(t)) - \sqrt{\varepsilon} \lambda \partial_x \bar{u}(t, x(t)) \quad (3.24)$$

is continuous at the interface. The derivation of (3.24) at the boundary will be detailed in the separate Sec. III B 1 for the reader’s convenience.

Approximating the derivative at first order with respect to η_1 and η_2 , respectively, we have

$$\begin{aligned} P(t, x_1(t)) - \sqrt{\varepsilon} \lambda \frac{\bar{u}_1(t, x_1(t)) - \bar{u}(t, x(t))}{\eta_1(t)} \\ = P(t, x_2(t)) - \sqrt{\varepsilon} \lambda \frac{\bar{u}(t, x(t)) - \bar{u}_2(t, x_2(t))}{\eta_2(t)} \\ + \mathcal{O}(\eta_1 + \eta_2). \end{aligned} \quad (3.25)$$

Finally, substituting this expression in (3.23) and considering the limit for $\eta_1 + \eta_2 \rightarrow 0$, we obtain

$$P_1 - P_2 = \lambda \sqrt{\varepsilon} \frac{(\eta_1 + \eta_2)^2}{\eta_1 \eta_2} D_t \alpha_1(t). \quad (3.26)$$

Now, let us compute

$$\frac{\partial}{\partial t} (\alpha_1 \rho) + \nabla_x (\alpha_1 \rho \bar{u})$$

$$= \alpha_1 \frac{\partial \rho}{\partial t} + \rho \frac{\partial \alpha_1}{\partial t} + \alpha_1 \nabla_x (\rho \bar{u}) + (\rho \bar{u}) \cdot \nabla_x (\alpha_1). \quad (3.27)$$

Recalling the definition of the material derivative and using Equations (3.8)–(3.26), we obtain

$$\frac{\partial}{\partial t} (\alpha_1 \rho) + \nabla_x \cdot (\alpha_1 \rho \bar{u}) = \rho \frac{D}{Dt} (\alpha_1) = -\frac{1}{\tau} (P_2 - P_1), \quad (3.28)$$

where $\tau := \frac{\sqrt{\varepsilon} \lambda (\eta_1 + \eta_2)^2}{\rho \eta_1 \eta_2}$ is the relaxation rate.

Thus, the pressure relaxation process drives a volume variation which evolves according to (3.28). In particular, we observe that the pressure relaxation implies a volume transfer towards the gas with highest pressure, according to the relaxation parameter $\tau > 0$.

Remark 3.3. The macroscopic velocity $\bar{u}$ for each point (x, t) is given by (3.14), obtained from the kinetic equation as (2.19). Inside a region occupied only by one species p , the macroscopic velocity automatically reduces to the single-species macroscopic velocity $\bar{u}_p$.

Then, since we have conservation of the single-species mass and conservation of total momentum at the kinetic level, the derivation of (3.12c) and (3.12d) is obtained taking respectively $\varphi(v) = 1$, $m_p v$, averaging in space and summing over the index p , using Gauss and Leibniz rules and (3.28). We observe that, despite setting the number of species M to 2, the validity of these equations remains independent from the number of species. The equation for total mass conservation (3.12a) is a straightforward consequence of the conservation of single-species mass.

Finally, we would like to recover the equation for the relative velocity. Since the momentum exchange occurs at the interface between the two gases, the relative velocity constitutes a local quantity, therefore no spatial averaging procedure is required. Considering the test function $\varphi(v) = m_p v$ in the weak formulation (3.16), we obtain

$$\frac{\partial}{\partial t} (\rho_p \bar{u}_p) + \nabla_x \cdot (\rho_p \bar{u}_p \otimes \bar{u}_p + P_p) = \sum_{q \neq p} \mathbf{R}_{p,q}, \quad (3.29)$$

where $\mathbf{R}_{p,q}$ is the momentum exchange rate. Following the idea presented in Ref. [34], we shall compute explicitly $\mathbf{R}_{p,q}$ in the case of Maxwellian molecules and hard spheres molecules. To this aim, in Appendix A we compute the product of two local Maxwellians $\mathcal{M}_p(v) \mathcal{M}_q(w)$, whose expression depends on the center of mass $\mathcal{V}$ and relative velocities $|v - w|$. Then, assuming pseudo-Maxwellian molecules (constant kernel $\mathbf{B}$ independent from the species) or hard-spheres molecules (kernel of the form $\mathbf{B} = |u|$ independent from the species), the explicit computation described in A leads to the following expression for the momentum exchange rate:

$$\mathbf{R}_{p,q} = -\xi_{p,q} \rho_p \rho_q (\bar{u}_p - \bar{u}_q), \quad \xi_{p,q} \in \mathbb{R}, \quad (3.30)$$

where the coefficients $\xi_{p,q}$ satisfy the symmetric property $\xi_{p,q} = \xi_{q,p}$. We first notice that the computation can be done for general distribution function f_p and f_q , if we are considering pseudo-Maxwellian molecules. Indeed, for this particular choice, the interaction kernel does not depend on the deviation angle nor the relative velocity and the exchange rate can be

written using (2.13) and the expression for the moments as

$$\begin{aligned} \mathbf{R}_{p,q} &= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} m_p m_q f_p(v) f_q(v_*) (v - v_*) d\sigma dv dv_* \\ &= \rho_p \rho_q (\bar{u}_p - \bar{u}_q). \end{aligned} \quad (3.31)$$

For general interaction particle, the presence of the interaction kernel make the computation really insidious and their explicit expressions are given in the Appendix A.

Now we can rewrite explicitly Eq. (3.29) and subtract the equation for the other species, obtaining

$$\begin{aligned} &\frac{1}{\rho_1} \frac{\partial}{\partial t} (\rho_1 \bar{u}_1) - \frac{1}{\rho_2} \frac{\partial}{\partial t} (\rho_2 \bar{u}_2) \\ &+ \frac{1}{\rho_1} \nabla_x \cdot (\rho_1 \bar{u}_1 \otimes \bar{u}_1 + P_1) - \frac{1}{\rho_2} \nabla_x \cdot (\rho_2 \bar{u}_2 \otimes \bar{u}_2 + P_2) \\ &= \frac{\mathbf{R}_{1,2}}{\rho_1} - \frac{\mathbf{R}_{2,1}}{\rho_2} = -\xi (\rho_2 + \rho_1) (\bar{u}_1 - \bar{u}_2). \end{aligned} \quad (3.32)$$

We can rewrite the pressure term in terms of the internal energy and the phase enthalpy as

$$P_p = \rho_p (h_p - e_p), \quad (3.33)$$

where h_p is the phase enthalpy and e_p is the internal energy. Assuming a polytropic gas for which $P(\rho) = \rho^\gamma$, the following relation holds:

$$\partial_x P_p = \rho_p \partial_x h_p. \quad (3.34)$$

Indeed, for an ideal gas it holds $P = \rho e(\gamma - 1)$,

$$\frac{1}{\rho} \nabla_x P = \frac{\gamma}{\rho} \rho^{\gamma-1} \nabla_x \rho, \quad \partial_x h = \nabla_x \left(\frac{P}{\rho} + e \right) = \gamma \rho^{\gamma-2} \nabla_x \rho, \quad (3.35)$$

which leads to (3.34).

Therefore, using (3.30) and (3.33) and defining the quantity

$$\zeta := \xi (\rho_1 + \rho_2) \quad (3.36)$$

we recover the following equation in the one-dimensional case:

$$\frac{\partial}{\partial t} (\bar{u}_1 - \bar{u}_2) + \frac{\partial}{\partial x} \left(\frac{1}{2} \bar{u}_1^2 - \frac{1}{2} \bar{u}_2^2 + h_1 - h_2 \right) = -\zeta (\bar{u}_1 - \bar{u}_2). \quad (3.37)$$

Therefore, through a formal hydrodynamic limit of the multispecies Boltzmann equation when $\varepsilon \rightarrow 0$ we have obtained a model similar to the two-phase flow model introduced in Ref. [7].

Remark 3.4. In this work we assume that the gas is isentropic at the macroscopic level. This assumption considerably simplifies the dynamics and enables the derivation of the isentropic two-phase flow model proposed in Ref. [7], which is of interest in itself. The particular scaling used in (2.29) justifies the assumption that the process leading $u_p \rightarrow u_q$ is slow enough for the entropy $\mathcal{H}$ to be considered constant. Under this assumption, we show that each species separately behaves isentropically, namely

$$P_p \propto \rho_p^{\gamma_p}.$$

Indeed, when plugging the local Maxwellian function $\mathcal{M}_p$ inside the expression of the per-species entropy $\mathcal{H}_p$, we obtain

$$\begin{aligned} \mathcal{H}_p &= \int_{\mathbb{R}^d} \mathcal{M}_p \ln \mathcal{M}_p dv \\ &= n_p \ln n_p + \frac{d}{2} n_p \ln \left(\frac{m_p}{2\pi T_p} \right) \\ &\quad - \int_{\mathbb{R}^d} \mathcal{M}_p \frac{m_p}{2T_p} |\bar{u}_p - v|^2 dv, \end{aligned}$$

where the last quantity is the thermal energy. By dividing this expression by ρ_p to obtain the expression of the entropy per unit mass and by imposing its derivative to be constant in time, you retrieve

$$\begin{aligned} c_1 \frac{1}{T_p} \frac{dT_p}{dt} &= c_2 \frac{1}{\rho_p} \frac{d\rho_p}{dt} \Rightarrow T_p = \rho_p^{c_1/c_2} + \text{const} \\ \Rightarrow P_p &= n_p T_p I \propto \rho_p^{\gamma_p}, \end{aligned}$$

for $c_1, c_2 \in \mathbb{R}$, and $\gamma_p = \gamma_p(c_1, c_2) \in \mathbb{R}$, which must be properly defined, where we have used the relation $\rho_p = m_p n_p$.

In future work, we aim to remove the isentropic assumption, in order to investigate the hydrodynamic limit towards the full two-phase model [8] (two-velocity, two-pressure, two-temperature model), which requires additional equations for the energy.

1. Derivation of the continuous stress tensor at the interface

The idea is to obtain an expression for the stress tensor at the boundary separating two phases, inspired by the the compressible boundary layer equations derived from the Boltzmann equation in Ref. [48] (see also Ref. [49] for the incompressible case).

Let us focus on the thin boundary layer across the interface of Fig. 3 and let us introduce a Prandtl scaling. From Prandtl theory, we know that if the Knudsen number is $\mathcal{O}(\varepsilon)$ and the fluid is compressible, then the thickness of such a region can be assumed $\mathcal{O}(\sqrt{\varepsilon})$. For the sake of simplicity, we can assume that the interface is located at $x_D = 0$ and the species 1 moves in the region described by the half-space $x' = (x_1, \dots, x_{D-1})$ with $x_D < 0$. Let us rescale the independent variables by obtaining:

$$x' = x, \quad x'_D = \frac{x_D}{\sqrt{\varepsilon}}, \quad \text{and} \quad t' = t. \quad (3.38)$$

The rescaled Boltzmann equation reads as

$$\begin{aligned} \partial_t f_p + v' \cdot \nabla_{x'} f_p + \frac{1}{\sqrt{\varepsilon}} v_D \partial_{x_D} f_p \\ = \frac{1}{\varepsilon} \mathcal{Q}_{pp}(f_p, f_p) + \mathcal{Q}_{pq}(f_p, f_q), \end{aligned} \quad (3.39)$$

where the advection term in the D direction describes the effect of the boundary layer at the interface. Since the process is “local” across the interface, no spatial averaging procedure is performed.

By using the Chapman-Enskog expansion introduced before in the weak formulation of (3.39) and matching different powers of ε , the truncation at the 0th-order level needs $\mathcal{Q}_{pp} = 0$ (which implies f_p must be a local

Maxwellian) and

$$\frac{1}{\sqrt{\varepsilon}} \int_{\mathbb{R}^d} \varphi(v) v_D \partial_{x_D} (f_p^0 + \varepsilon f_p^1) dv = 0. \quad (3.40)$$

Since (3.40) is the only $1/\sqrt{\varepsilon}$ term, this implies

$$\int_{\mathbb{R}^d} \varphi(v) v_D \partial_{x_D} (f_p^0 + \varepsilon f_p^1) dv = 0. \quad (3.41)$$

Let us first take $\varphi(v) = m_p$ in (3.40) and sum over the species p , from which using (3.5) we have

$$\partial_{x_D} \left(\sum_p \rho_p \bar{u}_p^D \right) = 0, \quad (3.42)$$

where u^D represents the component of u in the D direction.

Then, taking $\varphi(v) = m_p v_D$ in (3.40) and summing over the species p , we obtain

$$\begin{aligned} \partial_{x_D} \left(\sum_p \rho_p (u_p^D)^2 + \sum_p P_p - \sum_p \sqrt{\varepsilon} \lambda \partial_{x_D} \bar{u}_p^D \right. \\ \left. - \sum_p \varepsilon \lambda \mathcal{D}_{x'}(\bar{u}_p) \right) = 0, \end{aligned} \quad (3.43)$$

where λ is the proper viscosity coefficient. The components depending on $\sqrt{\varepsilon}$ and ε are obtained as corrections in ε in the Chapman-Enskog expansion at the Navier-Stokes level. Indeed, as shown in Refs. [38,50], the conservation law at order 0 and the Hilbert's lemma leads to a first-order flux correction of the form $\varepsilon \operatorname{div}_x(\lambda \mathcal{D}(\bar{u}_p))$, where

$$\mathcal{D}(u) = \frac{1}{2} (\nabla_x u + (\nabla_x u)^T) - \frac{1}{3} (\nabla_x \cdot u) \operatorname{Id}, \quad (3.44)$$

namely $\mathcal{D}(\bar{u}_p)$ is the traceless part of the deformation tensor of $\bar{u}_p$. In the one-dimensional case it reduces to $\mathcal{D}(u) = \partial_x u$.

Let us focus on the expression (3.43) at the interface $x_D = 0$. We recall that the two species are separated; therefore, we can assume without loss of generality that the half-plane $x_D < 0$ is occupied by the species 1 and the half-plane $x_D > 0$ is occupied by the species 2. This implies that the partial momentum $\rho_2 u_2$ and the partial pressure P_2 , related to the species 2, are null in the half-plane $x_D < 0$ and vice versa. The first equation (3.42) implies

$$\rho_1(t, x(t)) \bar{u}_1(t, x(t)) = k = \rho_2(t, \tilde{x}(t)) \bar{u}_2(t, \tilde{x}(t)), \quad (3.45)$$

where $x_D < 0$ and $\tilde{x}_D > 0$.

By using this relation in the second equation (3.43) and truncating at first order in ε , we obtain

$$\begin{aligned} k (\bar{u}_1(t, x(t)) + P_1(t, x(t)) - \sqrt{\varepsilon} \lambda \frac{\partial \bar{u}_1(t, x(t))}{\partial x_D}) \\ = k \bar{u}_2(t, \tilde{x}(t)) + P_2(t, \tilde{x}(t)) - \sqrt{\varepsilon} \lambda \frac{\partial \bar{u}_2(t, \tilde{x}(t))}{\partial x_D}, \end{aligned} \quad (3.46)$$

where $x_D < 0$ and $\tilde{x}_D > 0$. By imposing continuity conditions of the normal velocity at the interface, we finally obtain the continuity of the stress tensor at the boundary at first order in ε , namely

$$P_1 - P_2 = \sqrt{\varepsilon} \lambda \partial_{x_D} \bar{u}_1(t, x(t)) - \sqrt{\varepsilon} \lambda \partial_{x_D} \bar{u}_2(t, x(t)). \quad (3.47)$$

2. Comparison with the Baer-Nunziato model

Baer-Nunziato-type models [1,46], differently to the model of two-phase compressible flow with two velocities and two pressures proposed in Ref. [7], are not in a conservative form. From a modeling point of view, the difference between these two approaches relies in the physical description of the phenomena: The conservative model has been proposed to deal with processes in which the thermal state of phases are almost in equilibrium state, while Baer-Nunziato-type models can take into account thermal nonequilibrium processes. To this aim, in this subsection we propose a comparison with the isentropic model derived above by considering Baer-Nunziato models in which thermal processes are ignored and the phases behavior is isentropic. As observed in Refs. [7,8,11], the one-dimensional versions of the models are very similar if properly rewritten. The main difference is the definition of an interfacial pressure, which provides different results in the modeling of the phenomena. The isentropic version of a simplified Baer-Nunziato model reads as follows:

$$\frac{\partial}{\partial t} (\alpha_1) + u_{\text{interface}} \partial_x (\alpha_1) = -\frac{1}{\tau} (P_2 - P_1), \quad (3.48a)$$

$$\frac{\partial}{\partial t} (\alpha_1 \rho_1) + \partial_x (\alpha_1 \rho_1 \bar{u}_1) = 0, \quad (3.48b)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_1 \rho_1 \bar{u}_1) + \partial_x (\alpha_1 \rho_1 \bar{u}_1^2 + \alpha_1 P_1) \\ = P_{\text{interface}} \partial_x \alpha_1 + \tilde{\zeta} (\bar{u}_2 - \bar{u}_1), \end{aligned} \quad (3.48c)$$

$$\frac{\partial}{\partial t} (\alpha_2 \rho_2) + \partial_x (\alpha_2 \rho_2 \bar{u}_2) = 0, \quad (3.48d)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_2 \rho_2 \bar{u}_2) + \partial_x (\alpha_2 \rho_2 \bar{u}_2^2 + \alpha_2 P_2) \\ = P_{\text{interface}} \partial_x \alpha_2 - \tilde{\zeta} (\bar{u}_2 - \bar{u}_1), \end{aligned} \quad (3.48e)$$

where $u_{\text{interface}}$ and $P_{\text{interface}}$ are the interfacial velocity and the interfacial pressure, respectively. The definition of interfacial velocity is the same for both models

$$u_{\text{interface}} = \bar{u} = \frac{\alpha_1 \rho_1 \bar{u}_1 + \alpha_2 \rho_2 \bar{u}_2}{\alpha_1 \rho_1 + \alpha_2 \rho_2}, \quad (3.49)$$

since the first equation (3.48a) could be easily derived from (3.12b) and (3.12c). Equations (3.48b)–(3.48d) are derived from the multispecies Boltzmann equation (3.15), as already shown for the conservative model.

The main difference lies in the equation for the balance of the single-species momentum. Indeed, by taking $\varphi(v) = m_p v$ in (3.16), followed by a spatial averaging procedure, we recover Eqs. (3.48c)–(3.48e), where $\tilde{\zeta}$ now is given by

$$\tilde{\zeta} := \frac{\xi}{\alpha_1 \alpha_2} \rho. \quad (3.50)$$

We conclude that both models could be derived from the multispecies Boltzmann equation (3.15) by considering different closure assumptions and different quantities of interest.

IV. CONCLUSIONS

In this paper we have formally derived the hyperbolic model introduced in Ref. [8] to reproduce the dynamics of two-phase flows, starting from a kinetic model for gas

mixtures. We have first investigated the properties of the multispecies Boltzmann equations and we have given a brief description of the behavior of the limit solution. We have then examined the hydrodynamic limit of the kinetic model under the regime of resonant intraspecies collisions, aiming to derive different equilibrium velocities for the two species. This choice allows to recover a description for two-phase flows at the macroscopic level, including the dynamics of the volume fraction and the treatment of the interface. We have kept an isentropic closure assumption on the pressure term in order to recover the original model. This assumption could be weakened in future works, leading to different macroscopic equations for multiphase flows, see for instance [51].

Several new directions could be pursued. The idea is to develop an asymptotic-preserving numerical scheme for the stiff kinetic model (3.15). This will enable numerical simulations, to provide a comparison between the behavior of the kinetic solution and that of the macroscopic equations (3.12a)–(3.12e) in the limit $\varepsilon \rightarrow 0$. Further, we could extend this strategy to more complex kinetic models, taking into account Boltzmann equations with different type of collisions, such as mixtures of gases undergoing inelastic collisions [52].

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No conflict of interest is extant in the present work.

DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX A: COMPUTATION OF THE MOMENTUM EXCHANGE RATE FOR HARD-SPHERES MOLECULES

We compute here the momentum exchange rate $\mathbf{R}_{p,q}$, describing the change in momentum for the species p due to the interactions with the other species q . We partially follow Refs. [20,53] and the more recent paper [54]. We assume a collision kernel $\mathbf{B}$ independent from the species. Since we are interested in an approximation of the exchange rate in the limit for $\varepsilon \rightarrow 0$, it is reasonable to consider f_p and f_q as two Maxwellian distribution functions. In particular we can write the exchange rate in the following form:

$$\mathbf{R}_{p,q} = \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}} m_p m_q \mathcal{M}_p(v) \mathcal{M}_q(v_*) (v - v_*) \mathbf{B}(|v - v_*|, \cos \theta) d\sigma dv dv_*. \quad (\text{A1})$$

Let us consider the product of two local Maxwellians,

$$\mathcal{M}_p(v) \mathcal{M}_q(v_*) = n_p \left(\frac{m_p}{2\pi \bar{T}} \right)^{\frac{d}{2}} \exp \left(-\frac{m_p}{2\bar{T}} |\bar{u}_p - v|^2 \right) n_q \left(\frac{m_q}{2\pi \bar{T}} \right)^{\frac{d}{2}} \exp \left(-\frac{m_q}{2\bar{T}} |\bar{u}_q - v_*|^2 \right). \quad (\text{A2})$$

We introduce the following relative center of mass with respect to the velocities at the equilibrium. We can define

$$\mathcal{W} = \frac{m_p \bar{u}_p + m_q \bar{u}_q}{m_p + m_q} - \mathcal{V}, \quad (\text{A3})$$

where $\mathcal{V}$ is the center of mass defined in (2.5). Now, we can rewrite

$$\begin{aligned}\bar{u}_p - v &= \mathcal{W} + \frac{m_q}{m_p + m_q}[(\bar{u}_p - v) - (\bar{u}_q - v_*)], \\ \bar{u}_q - v_* &= \mathcal{W} + \frac{m_p}{m_p + m_q}[(\bar{u}_q - v_*) - (\bar{u}_p - v)].\end{aligned}$$

Using this new variable, we can rewrite the product (A2) as

$$\mathcal{M}_p(v) \mathcal{M}_q(v_*) = K_{pq} \exp\left(-\frac{|\mathcal{W}|^2}{\mu_{pq}} - \frac{|(v - v_*) - (\bar{u}_p - \bar{u}_q)|^2}{\gamma_{pq}}\right), \quad (\text{A4})$$

where

$$K_{pq} = n_p n_q \frac{(m_p m_q)^{\frac{d}{2}}}{(2\pi \bar{T})^d}, \quad \mu_{pq} = \frac{2\bar{T}}{(m_p + m_q)}, \quad \gamma_{pq} = \frac{2(m_p + m_q)\bar{T}}{m_p m_q}. \quad (\text{A5})$$

Now we can perform the integral with respect the new variables $\mathcal{W}$ and $w := v - v_*$, observing that the Jacobian of the transformation is unitary, which implies $dv dv_* = dw d\mathcal{W}$. Hence, integrating first over $d\mathcal{W}$,

$$\mathbf{R}_{p,q} = \pi^{\frac{d}{2}} \mu_{pq}^d K_{pq} m_p m_q \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} \mathbf{B}(|w|, \cos \theta) w \exp\left(-\frac{|w - (\bar{u}_p - \bar{u}_q)|^2}{\gamma_{pq}}\right) d\sigma dw. \quad (\text{A6})$$

We now restrict our analysis to the hard-spheres case for $d = 3$, where the interaction kernel is

$$\mathbf{B}(|w|, \cos \theta) = |w|, \quad (\text{A7})$$

from which we obtain

$$\mathbf{R}_{p,q} = 2\pi^{\frac{5}{2}} \mu_{pq}^3 K_{pq} m_p m_q \int_{\mathbb{R}^3} |w| w \exp\left(-\frac{|w - (\bar{u}_p - \bar{u}_q)|^2}{\gamma_{pq}}\right) dw. \quad (\text{A8})$$

Let us rewrite w in spherical coordinates

$$w = |w|(\sin \varphi \cos \psi, \sin \varphi \sin \psi, \cos \varphi). \quad (\text{A9})$$

Then,

$$\begin{aligned}I_{p,q} &:= \int_{\mathbb{R}^3} |w| w \exp\left(-\frac{|w - (\bar{u}_p - \bar{u}_q)|^2}{\gamma_{pq}}\right) dw \\ &= \int_0^\pi \int_0^{2\pi} \int_0^\infty |w|^3 \hat{w} \exp\left(-\frac{|w - (\bar{u}_p - \bar{u}_q)|^2}{\gamma_{pq}}\right) \sin \varphi d\varphi d\psi d|w| \\ &= 2\pi \hat{e}_3 \int_0^\pi \int_0^\infty |w|^4 \exp\left(-\frac{|w - (\bar{u}_p - \bar{u}_q)|^2}{\gamma_{pq}}\right) \cos \varphi \sin \varphi d\varphi d|w|,\end{aligned}$$

where $\hat{w} = w/|w|$ and $\hat{e}_3$ could be chosen in the direction of $\bar{u}_p - \bar{u}_q$.

Introducing the first change of variable

$$\alpha = (\bar{u}_p - \bar{u}_q) \cos \varphi, \quad \beta = |w|, \quad v = \bar{u}_p - \bar{u}_q, \quad (\text{A10})$$

the integral becomes

$$I_{p,q} = \frac{2\pi}{|v|^3} v \exp\left(-\frac{v^2}{\gamma_{pq}}\right) \int_{-v}^v \int_0^\infty \beta^4 \alpha \exp\left(-\frac{\beta^2}{\gamma_{pq}} - \frac{2\beta\alpha}{\gamma_{pq}}\right) d\alpha d\beta. \quad (\text{A11})$$

Now we introduce another change of variable

$$\eta = \beta + \alpha, \quad (\text{A12})$$

in order to rewrite $I_{p,q}$ as

$$I_{p,q} = \frac{2\pi}{|v|^3} v \exp\left(-\frac{v^2}{\gamma_{pq}}\right) \int_{-v}^v \int_0^\infty \alpha(\eta - \alpha)^4 \exp\left(-\frac{\eta^2}{\gamma_{pq}} + \frac{\alpha^2}{\gamma_{pq}}\right) d\alpha d\eta.$$

Let us consider the rescaled variables

$$\eta = \frac{\eta}{\sqrt{\gamma_{pq}}}, \quad \alpha = \frac{\alpha}{\sqrt{\gamma_{pq}}}.$$

Now, avoiding the label in γ_{pq} , we have

$$I_{p,q} = \frac{2\pi}{|v|^3} \gamma^{11/2} v \exp\left(-\frac{v^2}{\gamma}\right) \int_{-\frac{v}{\gamma}}^{\frac{v}{\gamma}} \int_0^\infty \alpha(\eta - \alpha)^4 \exp(-\eta^2 + \alpha^2) d\alpha d\eta.$$

We first perform the integration in $d\eta$,

$$\int_\alpha^\infty (\eta - \alpha)^4 \exp(-\eta^2) d\eta = \frac{1}{8} \sqrt{\pi} (3 + 12\alpha^2 + 4\alpha^4) \operatorname{erfc}(\alpha) - \frac{1}{4} \alpha \exp(-\alpha^2) (5 + 2\alpha^2),$$

where "erfc" is the complementary error function.

The final expression for $I_{p,q}$ is

$$\begin{aligned} I_{p,q} &= \frac{\pi}{4|v|^3} \gamma^{11/2} v e^{\left(-\frac{v^2}{\gamma}\right)} \left(-4\left(\frac{v}{\gamma}\right)^3 + 2\left(\frac{v}{\gamma}\right) - \sqrt{\pi} \left(4\left(\frac{v}{\gamma}\right)^4 + 4\left(\frac{v}{\gamma}\right)^2 - 1 \right) e^{\left(\frac{v}{\gamma}\right)^2} \operatorname{erf}\left(\frac{v}{\gamma}\right) \right) \\ &= \pi v \left[e^{\left(-\frac{v^2}{\gamma}\right)} \left(\gamma^{5/2} + \frac{\gamma^{9/2}}{2v^2} \right) - \sqrt{\pi} \left(v\gamma^{3/2} + \frac{\gamma^{7/2}}{v} - \frac{\gamma^{11/2}}{4v^3} \right) \operatorname{erf}\left(\frac{v}{\gamma}\right) \right]. \end{aligned}$$

We can conclude that

$$\mathbf{R}_{p,q} = \rho_p \rho_q (\bar{u}_p - \bar{u}_q) \Psi_{p,q},$$

$$\text{where } \Psi_{p,q} = \frac{(m_p m_q)^{\frac{d}{2}}}{\sqrt{\pi}(m_p + m_q)} \frac{I_{p,q}}{(\bar{u}_p - \bar{u}_q)}.$$

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