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# On the macroscopic/kinetic closure of balance laws

**Abstract.** This paper presents a review of the results which illustrate the interplay of macroscopic (continuum) approach and kinetic theory of gases in solving the closure problem. Continuum approach to the closure problem is based upon entropy principle, and it is limited since phenomenological coefficients cannot be explicitly determined. On the other hand, kinetic theory provides closed systems of equations as approximate solutions to the Boltzmann equation, but it is mainly limited to rarefied gases. Combined closure procedure, reviewed in this paper, proposes a systematic matching procedure in which advantages of both approaches are taken into account. It is illustrated by the classical examples of Navier-Stokes-Fourier system and 13 moments model, but also with novel applications to the multi-temperature mixture of Euler fluids.

**Keywords.** Extended thermodynamics, moment method, closure problem.

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# 1 - Introduction

Balance laws are the systems of partial differential equations which represent the physical laws. They are valid for all media, but they do not constitute a closed system of equations—unknown field quantities outnumber the available equations. Consequently, certain number of quantities, usually fluxes and source terms, should be expressed in terms of field variables (and their derivatives) by means of constitutive relations. In such a way the system of balance laws becomes closed.

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Typical example are the balance (conservation) laws of mass, momentum and energy in continuum thermomechanics [17]. In this case, the stress tensor and the heat flux, which are the non-convective fluxes of momentum and internal energy, respectively, are expressed in terms of velocity and temperature gradients in classical Navier-Stokes-Fourier model. These linear constitutive relations are compatible with an entropy inequality [12,17], but also comprise the material properties, viscosity and thermal conductivity, which cannot be explicitly determined within the framework of continuum approach. To estimate them one has either to use the experimental evidence or, if appropriate, to take the results of more refined theories which describe the material at a smaller scale. An example of the latter approach are the estimates provided by the kinetic theory of gases that are valid for rarefied gases [21].

The closure problem becomes more delicate in the case of non-equilibrium processes described by the higher order models. A particular example of interest for this study is rational extended thermodynamics (RET)—a continuum theory that provides a systematic procedure for derivation of governing equations in the form of balance laws [30, 39, 40]. It extends the list of field variables by the fluxes (and their fluxes) and builds up the model which efficiently captures the non-equilibrium behavior. At the same time, it preserves dissipative character of the model through its compatibility with entropy inequality. It turned out that RET balance laws are fully compatible with Grad's moment equations in the kinetic theory of gases [11], although they are derived and closed in a completely different manner. Namely, Grad's equations are transfer equations for the moments of approximate velocity distribution function. Nevertheless, a full correspondence between these models may be established, and so-called phenomenological coefficients in RET may be determined by means of kinetic moment equations, albeit in the linear approximation of the source terms. It has to be noted that phenomenological coefficients in the models restricted to 13/14 moments can be related to classical transport coefficients—viscosity and thermal conductivity—by means of appropriate asymptotic procedure, the so-called Maxwellian iteration [18, 21, 39].

The closure problem in macroscopic (continuum) approach faces serious limitations when it takes into account higher order moments, or other variables which describe the non-equilibrium state of the medium. An example for that is a multi-temperature (MT) model of mixtures developed within RET, in which the balance laws contain the source terms with phenomenological coefficients/matrices [**37**]. Neither can they be determined within the macroscopic approach, nor one can rely upon experimental evidence because it is scarce.

Intention of this paper is to present the review of results that can be regarded as a toolbox for macroscopic/kinetic closure of balance laws. The core [3]

idea is to match the macroscopic equations for continuous media with relevant approximate solution of the Boltzmann equation(s). Although the idea possesses a flavor of generality, it still does not have a general structure and it will be presented through the sequence of examples. This will start with a classical matching of the Navier-Stokes-Fourier model of fluid dynamics with the Chapman-Enskog expansion in the kinetic theory. Further, the matching of 13 moments model of RET and the corresponding Grad's moment equations will demonstrate the nucleus of the closure problem in higher order models. Finally, recently obtained results [27,34] about macroscopic/kinetic closure in mixtures will be presented.

# 2 - Classical results: the Navier-Stokes-Fourier model

In continuum theory, the classical governing equations consist of the conservation laws of mass, momentum and energy:

$$(2.1) \qquad \frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_j}(\rho v_j) = 0,$$
$$(2.1) \qquad \frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_i v_j - t_{ij}) = 0,$$
$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho v^2 + \rho\varepsilon\right) + \frac{\partial}{\partial x_j}\left\{\left(\frac{1}{2}\rho v^2 + \rho\varepsilon\right)v_j - t_{ij}v_i + q_j\right\} = 0,$$

where  $\rho(t, \mathbf{x})$ ,  $v_i(t, \mathbf{x})$  and  $\varepsilon(t, \mathbf{x})$  are the fields of mass density, velocity and specific internal energy, all regarded as functions of time  $t \in \mathbb{R}$  and space variable  $\mathbf{x} \in \mathbb{R}^3$ , and  $t_{ij}$  and  $q_i$  are components of the stress tensor and the heat flux, respectively. Equations (2.1) are given in Cartesian form and summation convention is assumed throughout the paper.

Stress tensor is usually expressed as a sum of the spherical tensor proportional to thermodynamic pressure p and viscous stress  $\sigma_{ij}$ :

(2.2) 
$$t_{ij} = -p\,\delta_{ij} + \sigma_{ij}.$$

Thermodynamic pressure p and specific internal energy  $\varepsilon$  determined as functions of mass density  $\rho$  and temperature T through thermal and caloric equations of state:

(2.3) 
$$p = p(\rho, T), \quad \varepsilon = \varepsilon(\rho, T).$$

If equations of state (2.3) are given beforehand, then appropriate constitutive relations for the viscous stress tensor  $\sigma_{ij}$  and the heat flux  $q_i$  are needed for the closure of equations (2.1). In the sequel attention will be restricted to the rarefied monatomic gases, which implies that the trace of the viscous stress tensor vanishes,  $\sigma_{kk} = 0$ . Denoting by  $\sigma_{\langle ij \rangle}$  the traceless part of the viscous stress tensor, we have:

$$\sigma_{\langle ij\rangle} := \sigma_{ij} - \frac{1}{3}\sigma_{kk}\,\delta_{ij} = \sigma_{ij}.$$

To derive the Navier-Stokes-Fourier model of continuum we shall rely on thermodynamic constitutive theory which requires that governing equations should be compatible with the entropy balance law:

(2.4) 
$$\frac{\partial}{\partial t}(\rho s) + \frac{\partial}{\partial x_j}\left(\rho s v_j + \frac{q_j}{T}\right) = \Sigma,$$

where s is the specific entropy and  $\Sigma$  is the entropy production rate. More precisely, constitutive functions should be chosen in such a form that entropy production is non-negative,  $\Sigma \geq 0$ , for any thermodynamic process. Starting from the assumption of local thermodynamic equilibrium [12], i.e. transforming the Gibbs relation and using the governing equations (2.1), one obtains the following form of the entropy production:

(2.5) 
$$\Sigma = -\frac{q_j}{T^2} \frac{\partial T}{\partial x_j} + \sigma_{\langle ij \rangle} D_{\langle ij \rangle} \ge 0, \quad D_{ij} := \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right),$$

where  $D_{\langle ij\rangle} \equiv \partial v_{\langle i}/\partial x_{j\rangle}$  is the traceless part of the symmetrized velocity gradient tensor  $D_{ij}$ . The simplest form of constitutive functions which is compatible with inequality (2.5) is the linear one:

(2.6) 
$$\sigma_{\langle ij\rangle} = 2\mu \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \quad q_j = -\kappa \frac{\partial T}{\partial x_j},$$

where phenomenological coefficients  $\mu$  and  $\kappa$  must satisfy the following inequalities:

(2.7) 
$$\mu \ge 0, \quad \kappa \ge 0.$$

They have a physical meaning of shear viscosity and thermal conductivity, respectively.

With inequalities (2.7) we reach the limit of the continuum approach. Phenomenological coefficients  $\mu$  and  $\kappa$  cannot be determined more precisely within its framework. To obtain their particular values, one has to refer to experimental data, or to rely on some more refined theoretical approach which may

provide sufficiently accurate approximation. In the case of rarefied gases, kinetic theory fits in the latter framework and we shall pursue in that direction in the sequel.

Kinetic description of a rarefied gas relies on the velocity distribution function  $f(t, \mathbf{x}, \boldsymbol{\xi})$  which determines the number of particles in the elementary phase space volume  $(d\mathbf{x}, d\boldsymbol{\xi})$  around the point  $(\mathbf{x}, \boldsymbol{\xi})$ , where  $\boldsymbol{\xi} \in \mathbb{R}^3$  is the particle velocity. Its evolution is determined by the Boltzmann equation:

(2.8) 
$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} = Q(f, f)(\boldsymbol{\xi}),$$

[5]

where Q(f, f) is the collision operator. Since particle velocity  $\boldsymbol{\xi}$  is the only microscopic variable, Boltzmann equation (2.8) describes behavior of monatomic gases. Equilibrium state of the gas  $f_E$  is the one which satisfies the condition:

(2.9) 
$$Q(f_E, f_E) = 0.$$

It is determined by the Maxwellian distribution:

(2.10) 
$$f_E = \frac{\rho}{m} \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left\{-\frac{|\boldsymbol{\xi} - \mathbf{v}|^2}{2(k_B/m)T}\right\},$$

where mass density  $\rho$ , velocity  $v_i$  and temperature T are defined as moments of the distribution function:

(2.11) 
$$\rho = \int_{\mathbb{R}^3} mf \,\mathrm{d}\boldsymbol{\xi}, \quad \rho v_i = \int_{\mathbb{R}^3} m\xi_i f \,\mathrm{d}\boldsymbol{\xi}$$
$$\frac{3}{2}\rho \frac{k_B}{m}T = \int_{\mathbb{R}^3} \frac{1}{2}m |\mathbf{C}|^2 f \,\mathrm{d}\boldsymbol{\xi} \equiv \rho\varepsilon,$$

where  $C_i = \xi_i - v_i$  is the peculiar velocity. Definitions (2.11) are universal they are valid for any distribution function f, not only  $f_E$ . Also, field variables  $\rho$ ,  $v_i$  and T may be the functions of  $(t, \mathbf{x})$ . In that case,  $f_E$  is called the local equilibrium distribution (local Maxwellian), and it will be denoted as  $f_M$  in the sequel. It satisfies the equilibrium condition (2.9),  $Q(f_M, f_M) = 0$ , but it does not satisfy the Boltzmann equation (2.8) for arbitrary field variables.

Due to existence of the collision invariants, functions  $\psi(\boldsymbol{\xi})$  for which the weak form of the collision operator vanishes,  $\int_{\mathbb{R}^3} \psi(\boldsymbol{\xi}) Q(f, f) d\boldsymbol{\xi} = 0$ , conservation laws (2.1) may be obtained from the Boltzmann equation as transfer equations of moments:

(2.12) 
$$\frac{\partial}{\partial t} \int_{\mathbb{R}^3} \psi f \,\mathrm{d}\boldsymbol{\xi} + \frac{\partial}{\partial x_i} \int_{\mathbb{R}^3} \xi_i \psi f \,\mathrm{d}\boldsymbol{\xi} = 0.$$

One may define the pressure tensor  $p_{ij} = -t_{ij}$  (the negative stress tensor) and the heat flux  $q_i$  as follows:

(2.13) 
$$p_{ij} = \int_{\mathbb{R}^3} mC_i C_j f \,\mathrm{d}\mathbf{C}, \quad q_i = \int_{\mathbb{R}^3} \frac{1}{2} m |\mathbf{C}|^2 C_i f \,\mathrm{d}\mathbf{C}.$$

However, like in the macroscopic case, the system is not closed. The strategy which leads to closure is based upon using the approximate velocity distribution function. This must take into account that pressure tensor and heat flux are non-equilibrium quantities—when evaluated in local equilibrium, for  $f = f_M$ , they reduce to:

(2.14) 
$$p_{ij} = \int_{\mathbb{R}^3} m C_i C_j f_M \, \mathrm{d}\mathbf{C} = p \, \delta_{ij}, \quad q_i = \int_{\mathbb{R}^3} \frac{1}{2} m |\mathbf{C}|^2 C_i f_M \, \mathrm{d}\mathbf{C} = 0,$$

where p is the thermodynamic pressure.

Approximate form of the velocity distribution function is found by the celebrated Chapman-Enskog method [9,21]. It is essentially an asymptotic method applied to a scaled Boltzmann equation:

(2.15) 
$$\frac{\partial f^{\epsilon}}{\partial t} + \xi_i \frac{\partial f^{\epsilon}}{\partial x_i} = \frac{1}{\epsilon} Q(f^{\epsilon}, f^{\epsilon}),$$

where the small parameter  $\epsilon = \text{Kn}$  is the Knudsen number—the ratio of the molecular mean free path and the macroscopic reference length. When  $\epsilon \ll 1$ , we are in the so-called hydrodynamic limit, and we seek for an asymptotic solution in the form:

(2.16) 
$$f^{\epsilon} = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \dots = \sum_{k=0}^{\infty} \epsilon^k f^{(k)}.$$

Peculiarity of the Chapman-Enskog method is that, apart from the Boltzmann equation and velocity distribution function, it also expands the macroscopic equations (2.1). As an outcome, zeroth approximation coincides with the local Maxwellian,  $f^{(0)} = f_M$ , whereas first approximation reads:

(2.17) 
$$f^{(1)} = f_M \left\{ -\frac{A}{T} C_i \frac{\partial T}{\partial x_i} - \frac{m}{k_B T} B C_i C_j \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right\}.$$

This approximate solution implies appropriate approximation of non-convective fluxes:

$$p_{\langle ij\rangle} \approx p_{\langle ij\rangle}^{(0)} + \epsilon p_{\langle ij\rangle}^{(1)}, \quad q_i \approx q_i^{(0)} + \epsilon q_i^{(1)},$$

where  $p_{\langle ij\rangle}^{(0)} = p \,\delta_{ij}$  and  $q_i^{(0)} = 0$  recover the local equilibrium values (2.14). It is remarkable that first approximation recovers the Navier-Stokes-Fourier constitutive relations (2.6):

(2.18) 
$$p_{\langle ij\rangle}^{(1)} = -2\mu \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \quad q_i^{(1)} = -\kappa \frac{\partial T}{\partial x_i}.$$

[7]

Nevertheless, phenomenological coefficients are now computed from the collision model:

$$\mu = \frac{5}{16} \frac{1}{\Omega^{(2,2)}} \sqrt{\frac{mk_B T}{\pi}}, \quad \kappa = \frac{75}{64} \frac{k_B}{m} \frac{1}{\Omega^{(2,2)}} \sqrt{\frac{mk_B T}{\pi}}$$

where  $\Omega^{(2,2)}$  is an integral which depends on the collision cross section. In such a way, shear viscosity  $\mu$  and thermal conductivity  $\kappa$  are explicitly determined once the collision model (cross section) is chosen.

The results presented here are classical and may be easily found in the literature. Nevertheless, they inherit some features that will be important in further analysis:

- (i) macroscopic (continuum) model is closed through compatibility with an entropy inequality;
- (ii) solution of the kinetic model (Boltzmann equation) is sought in approximate form;
- (iii) phenomenological coefficients are determined by matching of macroscopic and kinetic closures.

This pattern will be reproduced in the analysis in two forthcoming Sections.

## 3 - Extended thermodynamics and Grad's 13 moments model

Classical Navier-Stokes-Fourier model inherits a paradox of the infinite speed of pulse propagation [**30**]. This is a consequence of parabolic character of the governing system of partial differential equations. Removal of this paradox appeared independently in two different frameworks—rational extended thermodynamics and kinetic theory of gases—through the system of moment equations.

Common feature of the moment equations in either approach is that they

form a hierarchy of balance laws [7]:

$$(3.1)$$

$$\frac{\partial}{\partial t}F + \frac{\partial}{\partial x_k}F_k = 0,$$

$$\frac{\partial}{\partial t}F_{i_1} + \frac{\partial}{\partial x_k}F_{i_1k} = 0,$$

$$\frac{\partial}{\partial t}F_{i_1i_2} + \frac{\partial}{\partial x_k}F_{i_1i_2k} = P_{i_1i_2},$$

$$\vdots$$

$$\frac{\partial}{\partial t}F_{i_1\cdots i_n} + \frac{\partial}{\partial x_k}F_{i_1\cdots i_nk} = P_{i_1\cdots i_n},$$

$$\vdots$$

In (3.1)  $F_{i_1\cdots i_n}$  denotes the tensor of order n; F,  $F_{i_1}$ ,  $F_{i_1i_2}$ ,... denote the densities, while  $F_k$ ,  $F_{i_1k}$ ,  $F_{i_1i_2k}$ ,... are the corresponding fluxes;  $P_{i_1i_2}$ ,... denote the source (production) terms; indices  $i_1, \ldots, i_n, k \in \{1, 2, 3\}$ . The moment system (3.1) has nested structure—fluxes of order m become densities of order m + 1. Finally, the system of moment equations could be infinite.

Since the infinite system of balance laws like (3.1) is intractable, it is usually truncated at certain tensorial order, say n, which generates the closure problem. It is assumed, both in extended thermodynamics and kinetic theory, that unknown fluxes and source terms should be expressed as functions of densities, but not of their derivatives. If this is fulfilled, the finite system of moment equations will become a quasi-linear hyperbolic system of balance laws, at least in some region of the state space. In such a way, the speed of propagation of the pulses will be finite in that region. Main difference between macroscopic and kinetic approach lies in the closure method.

In macroscopic approach, developed in the framework of rational extended thermodynamics, closure procedure relies on two fundamental principles [30]: (i) invariance of the governing equations with respect to Galilean transformations, and (ii) entropy principle, i.e. compatibility with entropy balance law. The former restricts the velocity dependence of fluxes and production terms [36]. The latter is achieved through application of the method of multipliers [23]. Apart from ensuring compatibility with entropy balance laws, multipliers play the role of the so-called main field—a privileged set of field variables for which the system balance laws transform into symmetric form [7,38].

In extended thermodynamics, a hyperbolic system of 13 moments equations for a monatomic, viscous, heat-conducting gas consists of conservation laws of mass, momentum and energy:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &+ \frac{\partial}{\partial x_j} \left( \rho v_j \right) = 0, \\ (3.2) \qquad \frac{\partial}{\partial t} \left( \rho v_i \right) &+ \frac{\partial}{\partial x_j} \left( \rho v_j v_i + p \,\delta_{ij} - \sigma_{\langle ij \rangle} \right) = 0, \\ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho v^2 + \rho \varepsilon \right) &+ \frac{\partial}{\partial x_j} \left\{ \left( \frac{1}{2} \rho v^2 + \rho \varepsilon + p \right) v_j - \sigma_{\langle ij \rangle} v_i + q_j \right\} = 0, \end{aligned}$$

and balance laws for momentum and energy flux:

(3.3) 
$$\frac{\partial}{\partial t} \left\{ \rho \left( v_i v_j - \frac{1}{3} v^2 \delta_{ij} \right) - \sigma_{\langle ij \rangle} \right\} + \frac{\partial}{\partial x_k} F_{\langle ij \rangle k} = P^M_{\langle ij \rangle},$$
$$\frac{\partial}{\partial t} \left\{ \left( \frac{1}{2} \rho v^2 + \frac{5}{2} p \right) v_i + q_i - \sigma_{ij} v_j \right\} + \frac{\partial}{\partial x_k} F_{ppik} = P^M_{ppi}.$$

Galilean invariance [36] yields the following relation between the source terms:

(3.4) 
$$P^{M}_{\langle ij\rangle} = \hat{P}^{M}_{\langle ij\rangle}, \quad P^{M}_{ppi} = \hat{P}^{M}_{\langle ij\rangle}v_j + \hat{P}^{M}_{ppi}$$

where the hats denote velocity independent terms. On the other hand, the entropy balance law reads:

(3.5) 
$$\frac{\partial}{\partial t}(\rho s) + \frac{\partial}{\partial x_j}(\rho s v_j + \psi_j) = \Sigma,$$

and the non-convective entropy flux  $\psi_j$  is regarded as constitutive quantity [28]. Compatibility of the balance laws (3.2)-(3.3) with entropy balance law (3.5), ensured by the application of Liu's method of multipliers [7,23,38], yields the following structure of the entropy production:

(3.6) 
$$\Sigma = \frac{1}{2pT} \sigma_{\langle ij \rangle} \hat{P}^{M}_{\langle ij \rangle} - \frac{\rho}{5p^2T} q_i \hat{P}^{M}_{ppi} \ge 0.$$

The simplest way to satisfy the entropy inequality (3.6) for any thermodynamic process is to choose the macroscopic source terms as follows:

(3.7) 
$$\hat{P}^{M}_{\langle ij\rangle} = \frac{1}{\tau_{\sigma}}\sigma_{\langle ij\rangle}, \quad \hat{P}^{M}_{ppi} = -\frac{1}{\tau_{q}}q_{i},$$

where:

(3.8) 
$$\tau_{\sigma}(\rho,T) > 0, \quad \tau_{q}(\rho,T) > 0,$$

[9]

[10]

are the relaxation times and they play the role of phenomenological coefficients. Like in the case of Navier-Stokes-Fourier model where continuum approach led to (2.7), we cannot get deeper insight into the functional form of relaxation times (3.8). Therefore, we shall turn to the kinetic approach.

Equations in the hierarchy of moment equations (3.1) can be written in general form:

(3.9) 
$$\frac{\partial}{\partial t}F_{i_1\cdots i_n} + \frac{\partial}{\partial x_k}F_{i_1\cdots i_n k} = P_{i_1\cdots i_n}^K$$

where  $P^{K} = 0$ ,  $P_{i}^{K} = 0$  and  $P_{ii}^{K} = 0$  due to collision invariants. Densities, fluxes and source terms in (3.9) are defined as moments of the velocity distribution function in the following way:

(3.10) 
$$F_{i_1\cdots i_n} = \int_{\mathbb{R}^3} m\xi_{i_1}\cdots\xi_{i_n} f \,\mathrm{d}\boldsymbol{\xi},$$
$$F_{i_1\cdots i_nk} = \int_{\mathbb{R}^3} m\xi_k\xi_{i_1}\cdots\xi_{i_n} f \,\mathrm{d}\boldsymbol{\xi},$$
$$P_{i_1\cdots i_n}^K = \int_{\mathbb{R}^3} m\xi_{i_1}\cdots\xi_{i_n} Q(f,f) \,\mathrm{d}\boldsymbol{\xi}$$

The moment method proposed by Grad is based upon approximation of the velocity distribution function using Hermite polynomials. The same approximation, with even more intricate relation to RET, may be obtained through application of the maximum entropy principle [8, 14, 19, 22]. In the end, 13 moments approximation of the velocity distribution function reads [21]:

(3.11) 
$$f_{13} = f_M \left\{ 1 + \frac{2}{\rho} \left( \frac{m}{2kT} \right)^2 \left[ p_{\langle ij \rangle} C_i C_j + \frac{4}{5} q_i C_i \left( \frac{m}{2kT} |\mathbf{C}|^2 - \frac{5}{2} \right) \right] \right\},$$

where  $f_M$  is the local Maxwellian. Moment equations derived using (3.11) are equivalent to moment equations of RET—conservation laws have the same form as (3.2), with  $\sigma_{\langle ij \rangle}$  replaced with  $-p_{\langle ij \rangle}$ , and balance laws for the momentum and the energy flux read:

$$\frac{\partial}{\partial t} \left(\rho v_i v_j + p_{ij}\right) + \frac{\partial}{\partial x_k} \left\{\rho v_i v_j v_k + v_i p_{jk} + v_j p_{ki} + v_k p_{ij} + p_{ijk}\right\} = P_{ij}^K,$$

$$(3.12) \quad \frac{\partial}{\partial t} \left\{ \left(\frac{1}{2}\rho |\mathbf{v}|^2 + \rho\varepsilon\right) v_i + p_{ij} v_j + q_i \right\} + \frac{\partial}{\partial x_j} \left\{ \left(\frac{1}{2}\rho |\mathbf{v}|^2 + \rho\varepsilon\right) v_i v_j + v_i v_k p_{jk} + v_j v_k p_{ik} + \frac{1}{2}\rho |\mathbf{v}|^2 p_{ij} + q_i v_j + q_j v_i + p_{ijk} v_k + q_{ij} \right\} = Q_i^K.$$

Non-convective fluxes are defined as:

$$p_{ijk} = \int_{\mathbb{R}^3} mC_i C_j C_k f \,\mathrm{d}\mathbf{C}, \quad q_{ij} = \int_{\mathbb{R}^3} \frac{1}{2} m |\mathbf{C}|^2 C_i C_j f \,\mathrm{d}\mathbf{C}$$

It is a matter of simple computation and use of the relation  $2\rho\varepsilon = 3p$  to prove the equivalence of (3.12) and (3.3).

Kinetic source terms may be computed in nonlinear form [21] using (3.11). However, they are more frequently used in the form which is linear with respect to non-equilibrium field variables, pressure tensor and heat flux:

(3.13)  

$$P_{ij}^{K} = \int_{\mathbb{R}^{3}} m\xi_{i}\xi_{j}Q(f_{13}, f_{13}) d\boldsymbol{\xi} = -\frac{1}{\tau}p_{\langle ij\rangle},$$

$$Q_{i}^{K} = \frac{1}{2}\int_{\mathbb{R}^{3}} m|\boldsymbol{\xi}|^{2}\xi_{i}Q(f_{13}, f_{13}) d\boldsymbol{\xi} = -\frac{1}{\tau}p_{\langle ij\rangle}v_{j} - \frac{2}{3\tau}q_{i},$$

with relaxation time explicitly determined [21]:

(3.14) 
$$\tau = \frac{5m}{16\rho} \left(\frac{m}{\pi kT}\right)^{1/2} \frac{1}{\Omega^{(2,2)}}.$$

Simple comparison of (3.7) and (3.13) leads to the following relation:

(3.15) 
$$\tau_{\sigma} = \tau, \quad \tau_q = \frac{3}{2}\tau.$$

In such a way the 13 moments system is completely closed. As a final comment note that in derivation of the source terms (3.13) and relaxation time (3.14) no particular assumption about the collision cross section was used, keeping the results as general as possible like in Section 2.

Closure of the moment system (3.2)-(3.3), i.e. computation of the phenomenological coefficients  $\tau_{\sigma}$  and  $\tau_q$ , is facilitated by the approximate solution (3.11) of the Boltzmann equation. At first sight it may seem that everything is done within the kinetic framework, and that macroscopic approach is redundant. This impression is a bit misleading. The macroscopic source terms (3.7) were determined from (3.6) as the simplest way to satisfy the entropy inequality for all thermodynamic processes. The kinetic source terms were computed from a weak form of the collision operator, for approximate velocity distribution function, and obtained in the form (3.13) after linearization. This difference, and the procedure used to match the results of two approaches, will pave the way for further applications of the combined macroscopic/kinetic closure.

[11]

### 4 - Mixture of Euler rarefied gases

Mixtures are substances consisted of more than one identifiable constituent. Our attention will be restricted to the mixture of rarefied gases. When the mixture undergoes a non-equilibrium process, extended set of field variables is needed to properly describe the state of the system. In that case both RET and kinetic theory provide appropriate tools for such description, each in its own way.

Within the framework of RET a multi-temperature model is developed to capture non-equilibrium behavior of the mixture [37]. It is rooted in the rational thermodynamics of mixtures [30, 39, 40, 43] and multi-velocity mixture model already established in RET [29]. If the mixture consists of n constituents, the main premise is that the state of the mixture is determined by  $(\rho_{\alpha}, \mathbf{v}_{\alpha}, T_{\alpha})_{\alpha=1}^{n}$ —mass densities, velocities and temperatures of the species. Governing equations consist of mass, momentum and energy balances of the species [37]:

$$\begin{aligned} \frac{\partial \rho_{\alpha}}{\partial t} + \operatorname{div}(\rho_{\alpha}\mathbf{v}_{\alpha}) &= \tau_{\alpha}^{M}, \\ (4.1) \quad \frac{\partial}{\partial t}(\rho_{\alpha}\mathbf{v}_{\alpha}) + \operatorname{div}(\rho_{\alpha}\mathbf{v}_{\alpha}\otimes\mathbf{v}_{\alpha} - \mathbf{t}_{\alpha}) &= \mathbf{m}_{\alpha}^{M}, \\ \quad \frac{\partial}{\partial t}\left(\frac{1}{2}\rho_{\alpha}v_{\alpha}^{2} + \rho_{\alpha}\varepsilon_{\alpha}\right) + \operatorname{div}\left\{\left(\frac{1}{2}\rho_{\alpha}v_{\alpha}^{2} + \rho_{\alpha}\varepsilon_{\alpha}\right)\mathbf{v}_{\alpha} - \mathbf{t}_{\alpha}\mathbf{v}_{\alpha} + \mathbf{q}_{\alpha}\right\} = e_{\alpha}^{M}, \end{aligned}$$

where  $\tau_{\alpha}^{M}$ ,  $\mathbf{m}_{\alpha}^{M}$  and  $e_{\alpha}^{M}$  are the source terms which describe the interaction among the species. They must obey the axiom of conservation [43]:

(4.2) 
$$\sum_{\alpha=1}^{n} \tau_{\alpha}^{M} = 0, \quad \sum_{\alpha=1}^{n} \mathbf{m}_{\alpha}^{M} = \mathbf{0}, \quad \sum_{\alpha=1}^{n} e_{\alpha}^{M} = 0,$$

since the conservation laws for the mixture must be recovered. In the sequel it will be assumed that all the constituents are Euler rarefied gases in which viscous stresses and heat conduction are negligible:

(4.3) 
$$\mathbf{t}_{\alpha} = -p_{\alpha}\mathbf{I}, \quad \mathbf{q}_{\alpha} = \mathbf{0},$$

and that partial pressures  $p_{\alpha}$  and partial specific energies  $\varepsilon_{\alpha}$  obey thermal and caloric equations of state of ideal gases:

(4.4) 
$$p_{\alpha} = \rho_{\alpha} \frac{k_{\rm B}}{m_{\alpha}} T_{\alpha}, \quad \varepsilon_{\alpha} = \frac{k_{\rm B}}{m_{\alpha}(\gamma_{\alpha} - 1)} T_{\alpha}.$$

It will also be assumed that there are no chemical reactions among the species, which amounts to  $\tau_{\alpha}^{M} = 0, \ \alpha = 1, \dots, n$ . For clarity of further analysis definitions of mixture density  $\rho$  and velocity  $\mathbf{v}$  will be recalled:

(4.5) 
$$\rho = \sum_{\alpha=1}^{n} \rho_{\alpha}, \quad \rho \mathbf{v} = \sum_{\alpha=1}^{n} \rho_{\alpha} \mathbf{v}_{\alpha}.$$

Using  $(4.5)_2$  the diffusion velocities  $\mathbf{u}_{\alpha}$  are defined as follows:

$$\mathbf{u}_{\alpha} := \mathbf{v}_{\alpha} - \mathbf{v}$$

The essence of a closure problem for the multi-temperature model (4.1) is to determine the structure of source terms  $\mathbf{m}_{\alpha}$  and  $e_{\alpha}$ . To that end one must first impose the restriction which implies Galilean invariance of the governing equations [**36**, **37**]:

(4.7) 
$$\mathbf{m}_{b}^{M} = \hat{\mathbf{m}}_{b}^{M}, \quad e_{b}^{M} = \hat{e}_{b}^{M} + \hat{\mathbf{m}}_{b}^{M} \cdot \mathbf{v}, \quad b = 1, \dots, n-1,$$

where  $\hat{\mathbf{m}}_b$  and  $\hat{e}_b$  are velocity independent parts of the source terms. Furthermore, application of the entropy principle with the aid of Liu's method of multipliers [7,23,38] leads to the following form of entropy production [37]:

(4.8) 
$$\Sigma = -\sum_{b=1}^{n-1} \left( \frac{\mathbf{u}_b}{T_b} - \frac{\mathbf{u}_n}{T_n} \right) \cdot \hat{\mathbf{m}}_b^M - \sum_{b=1}^{n-1} \left( -\frac{1}{T_b} + \frac{1}{T_n} \right) \hat{e}_b^M \ge 0.$$

Entropy inequality (4.8) may be satisfied for any thermodynamic process if the source terms have the form [37, 41]:

(4.9) 
$$\hat{\mathbf{m}}_{b}^{M} = -\sum_{c=1}^{n-1} \psi_{bc}(\mathbf{w}) \left(\frac{\mathbf{u}_{c}}{T_{c}} - \frac{\mathbf{u}_{n}}{T_{n}}\right), \quad \hat{e}_{b}^{M} = -\sum_{c=1}^{n-1} \theta_{bc}(\mathbf{w}) \left(-\frac{1}{T_{c}} + \frac{1}{T_{n}}\right).$$

In (4.9)  $\psi_{bc}(\mathbf{w})$  and  $\theta_{bc}(\mathbf{w})$  are positive semi-definite matrix functions of objective quantities  $\mathbf{w} = (\rho_{\alpha}, \mathbf{u}_{\alpha}, T_{\alpha})_{\alpha=1}^{n}$ . They have a role of phenomenological coefficients.

At this stage we are facing the most delicate part of the closure problem. In Navier-Stokes-Fourier model and in 13 moments model matching of macroscopic and kinetic phenomenological coefficients was a matter of choice. They can be determined from the experimental evidence as well. However, in the case of multi-temperature mixture experimental data do not exist, or may be found for very specific processes only. Therefore, there is no other way to estimate phenomenological coefficients than to match them with kinetic multi-temperature model.

[14]

The kinetic model of mixtures that will be presented is the one for polyatomic gases to which much attention was devoted recently [13]. In that model, the state of each species is described by its own velocity distribution function  $f_{\alpha}(t, \mathbf{x}, \boldsymbol{\xi}, I)$ , where  $I \in \mathbb{R}_+$  is the lumped parameter bringing the information about all internal degrees of freedom of the molecule. The dynamics is described by the system of Boltzmann equations:

(4.10) 
$$\frac{\partial f_{\alpha}}{\partial t} + \xi_i \frac{\partial f_{\alpha}}{\partial x_i} = \sum_{\beta=1}^n Q_{\alpha\beta}(f_{\alpha}, f_{\beta})(\boldsymbol{\xi}, I),$$

in which  $Q_{\alpha\beta}(f_{\alpha}, f_{\beta})$  are the collision operators of non-reactive collisions. Densities are defined as moments of the velocity distribution functions in the following way:

(4.11) 
$$\rho_{\alpha} = \int_{\mathbb{R}^{3} \times \mathbb{R}_{+}} m_{\alpha} f_{\alpha} \varphi_{\alpha}(I) dI d\boldsymbol{\xi},$$
$$\rho_{\alpha} \mathbf{v}_{\alpha} = \int_{\mathbb{R}^{3} \times \mathbb{R}_{+}} m_{\alpha} \boldsymbol{\xi} f_{\alpha} \varphi_{\alpha}(I) dI d\boldsymbol{\xi},$$
$$\frac{1}{2} \rho_{\alpha} v_{\alpha}^{2} + \rho_{\alpha} \varepsilon_{\alpha} = \int_{\mathbb{R}^{3} \times \mathbb{R}_{+}} \left(\frac{1}{2} m_{\alpha} |\boldsymbol{\xi}|^{2} + I\right) f_{\alpha} \varphi_{\alpha}(I) dI d\boldsymbol{\xi},$$

where  $\varphi_{\alpha}(I) dI$  is the measure of internal degrees of freedom. Similarly, the source terms are determined as:

(4.12)  
$$\mathbf{m}_{\alpha}^{K} = \sum_{\beta \neq \alpha} \int_{\mathbb{R}^{3} \times \mathbb{R}_{+}} m_{\alpha} \boldsymbol{\xi} Q_{\alpha\beta}(f_{\alpha}, f_{\beta}) \varphi_{\alpha}(I) dI d\boldsymbol{\xi},$$
$$e_{\alpha}^{K} = \sum_{\beta \neq \alpha} \int_{\mathbb{R}^{3} \times \mathbb{R}_{+}} \left(\frac{1}{2} m_{\alpha} |\boldsymbol{\xi}|^{2} + I\right) Q_{\alpha\beta}(f_{\alpha}, f_{\beta}) \varphi_{\alpha}(I) dI d\boldsymbol{\xi},$$

To recover the system of balance laws (4.1) for the multi-temperature mixture of Euler gases one has to approximate the velocity distribution functions  $f_{\alpha}$ with local Maxwellians with different species velocities  $\mathbf{v}_{\alpha}$  and different species temperatures  $T_{\alpha}$  [4]:

(4.13) 
$$f_{\alpha M} = \frac{\rho_{\alpha}}{m_{\alpha}\zeta_{\alpha}(T_{\alpha})} \left(\frac{m_{\alpha}}{2\pi k_B T_{\alpha}}\right)^{3/2} e^{-\frac{1}{k_B T_{\alpha}} \left(\frac{m_{\alpha}}{2} |\boldsymbol{\xi} - \mathbf{v}_{\alpha}|^2 + I\right)}.$$

Nevertheless, the source terms  $\mathbf{m}_{\alpha}^{K}$  and  $e_{\alpha}^{K}$  have a functional form much more complicated than (4.9)—they are expressed in terms of Kummer confluent hypergeometric functions  $_{1}\tilde{F}_{1}(a, b, z)$  [34]. To illustrate, the source terms in the

momentum balance laws read:

(4.14) 
$$\mathbf{m}_{\alpha} = -\sum_{\beta \neq \alpha} \Omega_{\alpha\beta} \mathbf{m}_{\alpha\beta},$$

where

[15]

$$\Omega_{\alpha\beta} = \mathbb{K}_* \mathbb{K}_{\alpha\beta} \frac{n_\alpha n_\beta k_B^{-(d_\alpha+d_\beta)}}{\Gamma[d_\alpha+1]\Gamma[d_\beta+1]} \frac{8\pi\mu_{\alpha\beta}}{s_{\alpha\beta}+5} \Gamma\left[\frac{s_{\alpha\beta}+3}{2}\right],$$

and

$$\mathbf{m}_{\alpha\beta} = (\mathbf{u}_{\alpha} - \mathbf{u}_{\beta}) T_{\alpha}^{-d_{\alpha}} T_{\beta}^{-d_{\beta}} \\ \times \left( \frac{2k_{B}T_{\alpha}}{m_{\alpha}} + \frac{2k_{B}T_{\beta}}{m_{\beta}} \right)^{s_{\alpha\beta}/2} e^{-\left(\frac{2k_{B}T_{\alpha}}{m_{\alpha}} + \frac{2k_{B}T_{\beta}}{m_{\beta}}\right)^{-1} |\mathbf{u}_{\alpha} - \mathbf{u}_{\beta}|^{2}} \\ \times {}_{1}\tilde{F}_{1} \left( \frac{s_{\alpha\beta} + 5}{2}, \frac{5}{2}, \left(\frac{2k_{B}T_{\alpha}}{m_{\alpha}} + \frac{2k_{B}T_{\beta}}{m_{\beta}}\right)^{-1} |\mathbf{u}_{\alpha} - \mathbf{u}_{\beta}|^{2} \right).$$

with  $n_{\alpha}$  being the number densities,  $\mu_{\alpha\beta}$  the reduced masses,  $d_{\alpha}$  parameters related to the ratios of specific heats;  $s_{\alpha\beta}$  is the parameter from the cross section. Constituent-related constant  $\mathbb{K}_{\alpha\beta}$  has the form

$$\mathbb{K}_{\alpha\beta} = \frac{m_0^2}{\rho_0^2} (k_B T_0)^{d_\alpha + d_\beta} \left(\frac{k_B}{\mu_{\alpha\beta}} T_0\right)^{-\frac{s_{\alpha\beta}}{2}},$$

where subscript 0 indicates the values of average quantities (mass, density and temperature) in a reference state, while  $\mathbb{K}_*$  is a common factor securing the proper dimension (see [27, 34] for details).

It is inevitable that matching of the source terms in RET and kinetic model is not straightforward. The way out of the problem lies in the fact that both models describe the same physical object and that their predictions should match at least in some region of the state space of macroscopic variables/moments. It is reasonable to expect that matching region lies in some neighborhood of the mixture local equilibrium, i.e. close to the state in which all species have the same velocity  $\mathbf{v}$  and the same temperature T. To that end the following strategy is proposed [27]:

(1) Linearize the RET source terms (4.9) in the neighborhood of mixture local equilibrium  $\mathbf{w}^0 = (\rho_\alpha, \mathbf{0}, T)_{\alpha=1}^n$ , where  $\mathbf{w} = (\rho_\alpha, \mathbf{u}_\alpha, T_\alpha)_{\alpha=1}^n$ :

(4.15)  
$$\hat{\mathbf{m}}_{b}^{M} \approx -\sum_{c=1}^{n-1} \psi_{bc}(\mathbf{w}^{0}) \left(\frac{\mathbf{u}_{c} - \mathbf{u}_{n}}{T}\right),$$
$$\hat{e}_{b}^{M} \approx -\sum_{c=1}^{n-1} \theta_{bc}(\mathbf{w}^{0}) \left(\frac{T_{c} - T_{n}}{T^{2}}\right).$$

[16]

- (2) Linearize the kinetic source terms (4.12) in the neighborhood of the same state  $\mathbf{w}^0$ . The resulting functional form will be the same as (4.15), albeit with explicitly computed phenomenological coefficients  $\psi_{bc}^K(\mathbf{w}^0)$  and  $\theta_{bc}^K(\mathbf{w}^0)$ .
- (3) Plug the kinetic phenomenological coefficients, computed in step (2), back into macroscopic source terms (4.9) to obtain:

(4.16)  

$$\hat{\mathbf{m}}_{b}^{M} = -\sum_{c=1}^{n-1} \psi_{bc}^{K}(\mathbf{w}^{0}) \left(\frac{\mathbf{u}_{c}}{T_{c}} - \frac{\mathbf{u}_{n}}{T_{n}}\right),$$

$$\hat{e}_{b}^{M} = -\sum_{c=1}^{n-1} \theta_{bc}^{K}(\mathbf{w}^{0}) \left(-\frac{1}{T_{c}} + \frac{1}{T_{n}}\right).$$

This is the final form of the source terms obtained by means of macroscopic/kinetic closure.

Explicit form of the kinetic phenomenological coefficients is [27]:

(4.17)

$$\psi_{bc}(\mathbf{w}^{0}) = \begin{cases} -\frac{2}{3}T\,\mu_{bc}\,K_{bc}^{\psi}, & b \neq c, \\ \frac{2}{3}T\sum_{\substack{\ell=1\\\ell\neq b}}^{n}\mu_{b\ell}K_{b\ell}^{\psi}, & b = c, \end{cases} \qquad \theta_{bc}(\mathbf{w}^{0}) = \begin{cases} -k_{\mathrm{B}}T^{2}K_{bc}^{\theta}, & b \neq c, \\ k_{\mathrm{B}}T^{2}\sum_{\substack{\ell=1\\\ell\neq b}}^{n}K_{b\ell}^{\theta}, & b = c, \end{cases}$$

where

$$K^{\psi}_{\alpha\beta} = \mathbb{K}_* \mathbb{K}_{\alpha\beta} \kappa^{\psi}_{\alpha\beta} \frac{\rho_{\alpha}}{m_{\alpha}} \frac{\rho_{\beta}}{m_{\beta}} \mu^{-\frac{s_{\alpha\beta}}{2}}_{\alpha\beta} (k_{\mathrm{B}}T)^{-\left(d_{\alpha}+d_{\beta}\right)+\frac{s_{\alpha\beta}}{2}}, \quad K^{\theta}_{\alpha\beta} = \kappa^{\theta}_{\alpha\beta} K^{\psi}_{\alpha\beta},$$

and

$$\kappa_{\alpha\beta}^{\psi} = \frac{2^{\frac{s_{\alpha\beta}}{2}+4}\Gamma\left[\frac{s_{\alpha\beta}+3}{2}\right]}{s_{\alpha\beta}+5} \frac{\sqrt{\pi}}{\Gamma\left[d_{\alpha}+1\right]\Gamma\left[d_{\beta}+1\right]},$$
$$\kappa_{\alpha\beta}^{\theta} = \frac{2\left(s_{\alpha\beta}+5\right)}{s_{\alpha\beta}+7} \left(\frac{1}{s_{\alpha\beta}+3} + \frac{\mu_{\alpha\beta}}{m_{\alpha}+m_{\beta}}\right).$$

A reasonable question may be posed again, like in the previous Section: Why do we need macroscopic RET model when complete closure comes from the kinetic approach? The reason for combined macroscopic/kinetic closure is twofold. First, kinetic phenomenological coefficients,  $\psi_{bc}^{K}(\mathbf{w}^{0})$  and  $\theta_{bc}^{K}(\mathbf{w}^{0})$ , are good first approximation of the macroscopic ones,  $\psi_{bc}(\mathbf{w})$  and  $\theta_{bc}(\mathbf{w})$ , respectively. Second, macroscopic RET source terms are nonlinear, whereas kinetic source terms with phenomenological coefficients are linearized. Nonlinearity of the source terms still may provide better insight into non-equilibrium processes than the linear ones.

Finally, there is a question of advantage of the macroscopic model with respect to the kinetic (mesoscopic) one. Macroscopic models presented in this study were closed by means of matching with some of the approximate solution of the Boltzmann equation. Although there are breakthroughs in numerical procedures for the Boltzmann equation [10,20,31,32], numerical solution of the system of partial differential equations still can be regarded as more accessible than its kinetic counterpart.

## 5 - Conclusions and outlook

This paper presents a short review of the recent results focused on modelling non-equilibrium processes in rarefied gases and their mixtures. The emphasis was on similarity of macroscopic and kinetic models under certain reasonable physical assumptions, and consistent matching of dissipative mechanisms which yields combined macroscopic/kinetic closure. First, it was recalled the classical result which relates Navier-Stokes-Fourier continuum model to a hydrodynamic limit of the Boltzmann equation and asymptotic solution obtained by means of Chapman-Enskog method. Second, it was presented the relation between 13 moments model derived within rational extended thermodynamics, and the corresponding Grad's model-kinetic model yields explicit form of relaxation times of the source terms in linearized form. Finally, recent results on macroscopic/kinetic closure in the mixture of Euler fluids were presented. They revealed the method of matching the source terms which is generally applicable. Although it is based upon linearization around local equilibrium, kinetic phenomenological coefficients are used in the nonlinear macroscopic source terms, thus enhancing the validity of the kinetic model.

Further steps in application of the macroscopic/kinetic closure are already made. In a recent study [1] a general procedure for extension of rational thermodynamics of mixtures to higher order moments is developed. It was applied in details to the mixture of gases with dynamic pressure [35], and the macroscopic/kinetic closure procedure was applied to determine the phenomenological coefficients. It was also shown that in such a mixture cross-effects must be taken into account. Also, in [27] closed system of equations for ternary mixture was tested in the shock structure problem. Convincing qualitative results of the test problems reassured that macroscopic/kinetic closure yields

physically reliable model. In fact, the shock structure problem is a benchmark problem for testing the capability of the model of non-equilibrium processes [2, 5, 6, 24, 25, 26, 33, 42]. Therefore, it is natural to apply the proposed closure procedure to mixtures with higher order moments and test the validity of the model through the shock structure problem.

Promising results obtained in the higher order models strengthen the belief that macroscopic/kinetic closure procedure can be established as a framework for systematic development of macroscopic non-equilibrium models. Let us support this statement with more arguments. Even though kinetic approach describes the system at a finer scale, its behavior is observed through macroscopic variables, which are the moments of the distribution function. On the other hand, macroscopic models inherit the information about physical mechanisms that relate macroscopic observables. Developing a macroscopic model compatible with entropy inequality, and then computing the phenomenological coefficients from the approximate form of source terms seems to be a feasible strategy. Moreover, this strategy may not be limited to rarefied gases. Recent results on kinetic modelling of dense gases and phase transition [3, 15, 16] in conjunction with appropriate macroscopic model open the possibility to apply the macroscopic/kinetic closure procedure to other models of fluids.

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