

Kinetic Bhatnagar-Gross-Krook model for fast reactive mixtures and its hydrodynamic limit

M. Bisi, M. Groppi, and G. Spiga

Dipartimento di Matematica, Università di Parma, Viale G. P. Usberti 53/A, 43100 Parma, Italy

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A recently proposed consistent Bhatnagar-Gross-Krook-type approach for reversible bimolecular chemical reactions, well suited to deal with collision dominated gas mixtures in which mechanical and chemical relaxation times are of the same order of magnitude (fast reactions), is discussed. The model recovers essential features of the chemical process such as mass action law at equilibrium and reactive H theorem. The hydrodynamic limit, at both Euler and Navier-Stokes levels, is derived by a Chapman-Enskog procedure, in terms of the relevant hydrodynamic variables, and compared to the corresponding limits holding in the nonreactive and in the slowly reactive cases. In particular, results show that reactive corrections to transport coefficients cannot be neglected for fast reactions.

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I. INTRODUCTION

Kinetic approaches to chemically reacting gas mixtures are gaining interest in the scientific literature for several reasons, and a crucial motivation is the fact that they allow a rigorous derivation and justification for the most common macroscopic descriptions used in the hydrodynamic regime [1,2]. On the other hand, nonlinear chemical collision integrals of Boltzmann type have been proposed in a recent past at various different levels [3–6]. We shall restrict here for simplicity to the easiest one [3], which ignores nontranslational degrees of freedom, yet capturing the essentials of the reactive encounters. Such integral operators are definitely awkward to manage and simpler approximate models would be useful for practical applications. Relaxation time approximations of the type proposed by Bhatnagar, Gross, and Krook [7] and by Welander [8] (usually denoted as BGK models) seem to be the first natural candidates in that direction. In standard one-species gas dynamics such models prescribe relaxation toward a local equilibrium with a strength determined by a suitable characteristic time. But the procedure must be carefully devised in order to avoid well-known drawbacks which arise when treating a multispecies gas [9,10], as necessary in this work, since we will be dealing with the bimolecular reversible chemical reaction



In Eq. (1) each species A^s is endowed with a mass m^s and an energy of chemical bond E^s , and it is conventionally assumed that $\Delta E = -\sum_{s=1}^4 \lambda^s E^s > 0$, where the λ^s constitute the string of stoichiometric coefficients (1, 1, -1, -1).

We recall from [3,4] that the space of collision invariants is seven dimensional, and conserved quantities are mass in the independent pairs of species (1,3), (1,4), (2,4), momentum and total (kinetic plus chemical) energy. Collision equilibria are determined as the seven parameter family of local Maxwellians

$$f_M^s(\mathbf{v}) = n^s \left(\frac{m^s}{2\pi KT} \right)^{3/2} \exp \left[-\frac{m^s}{2KT} (\mathbf{v} - \mathbf{u})^2 \right] \quad s = 1, \dots, 4 \quad (2)$$

with \mathbf{u} and T standing for mass velocity and temperature of the mixture, and where number densities n^s must be related by the mass action law

$$\frac{n^1 n^2}{n^3 n^4} = \left(\frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \exp \left(\frac{\Delta E}{KT} \right), \quad (3)$$

in which use has been made of the reduced masses $\mu^{sr} = m^s m^r / (m^s + m^r)$. K denotes as usual the Boltzmann constant. We can also introduce the H -functional,

$$H[f] = \sum_{s=1}^4 \int f^s(\mathbf{v}) \log \left[\frac{f^s(\mathbf{v})}{(m^s)^3} \right] d\mathbf{v}, \quad (4)$$

and prove that H is a strict Lyapunov functional for stability of the equilibria given in Eq. (2) (H theorem).

Some relaxation models for reactive mixtures accounting for exchange of mass and of energy of chemical link have already been introduced in the literature [11–13]. In particular, the latter paper follows the consistent BGK strategy proposed in [10] for inert mixtures, which preserves positivity and indifferenciability principles, and resorts to a single BGK collision term for each species s ($s=1,2,3,4$), describing globally all binary interactions, mechanical (elastic) and chemical, with whatever other species. The approximate collision operator drifts the distribution function f^s toward a suitable local Maxwellian \mathcal{M}_s , characterized by macroscopic parameters, which are not the actual fields, moments of f^s (number density n^s , drift velocity \mathbf{u}^s , and temperature T^s), but remain disposable for the purposes of the method. The proposed machinery must rely on the explicit expressions of the exact Boltzmann exchange rates for mass, momentum, and energy of each species, which are available only for the collision model of Maxwell-type interactions [14] and in a physical regime of slow chemical reactions [15]. Within this domain of applicability, the model in [13] has proved effective

tive in investigating classical fluid-dynamic problems such as space homogeneous relaxation, shock wave structure, and Riemann problem.

It is clear, however, the need for a relaxation algorithm that can overcome the above restrictions capable to deal with general differential cross sections (with possible activation energy) and suitable for a regime of fast chemistry. In order to fill up this gap, a different strategy, still along the lines of [10], has been proposed in [16], and numerically applied in [17,18]. In this paper we intend to proceed further in such direction by investigating in particular one important aspect that was left as future work, namely, the hydrodynamic limit for small collision times of the present BGK equations (in the present frame, mechanical and chemical collision times are equally small). The analysis is based on the extension to a reactive mixture of the classical asymptotic Chapman-Enskog expansion, rather heavy already for inert mixtures [19,20], pushed up to first-order corrections in order to achieve (fast) reactive Navier-Stokes equations. This fast reactive scenario corresponds to the so called ‘‘equilibrium’’ regime of the classical thermodynamical literature [21], and the question of its hydrodynamic limit was addressed in [22] starting from reactive kinetic equations of Boltzmann type. Such an approach bears serious mathematical and technical difficulties related also to the solution of linearized integral equations with both mechanical and chemical operators.

On the other hand, the problem is of paramount importance for practical applications since, in many physical regimes, macroscopic-type partial differential equations involving the most meaningful observable quantities are adequate provided constitutive equations are accurate and reliable, and definitely much easier to deal with. In the classical thermodynamical literature (see for instance [23]) effects of the chemical reaction taking place in the mixture on transport coefficients are often neglected, and the reactive process is taken into account by additional contributions in the balance equations, which might be reaction sources (sinks), and, as peculiar in this chemical frame, an extra reactive scalar pressure [24]. Investigations such as the present one should then be useful in order to shed light on the above facts. Of course, it would be desirable that the conclusions of different theoretical approaches in different physical scenarios could be validated by experiments, but unfortunately authors are not aware of results or settings of this kind.

The article is organized as follows. After presenting in Sec. II the main features of the considered fast BGK model, the following sections are devoted to a detailed formal asymptotic analysis of the Chapman-Enskog type leading to closed macroscopic equations up to the Navier-Stokes level, which can be compared to analogous results obtained from BGK equations in the chemically neutral case [10], or from a Grad expansion technique for slowly reacting mixtures [25]. In particular, Sec. III deals with the generalities on the method and on the zero-order approximation, while Sec. IV analyzes the first-order corrections with the pertinent constitutive equations. Finally, results are summarized and briefly commented on in Sec. V.

II. BGK EQUATIONS

We recall and discuss here the main features of the relaxation-time approximation introduced in [16] for the

chemical reaction model worked out in [3]. Model kinetic equations read as

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \frac{\partial f^s}{\partial \mathbf{x}} = \nu_s (\mathcal{M}_s - f^s) \quad s = 1, \dots, 4, \quad (5)$$

where \mathcal{M}_s are the family of local Maxwellians

$$\mathcal{M}_s(\mathbf{v}) = \tilde{n}^s \left(\frac{m^s}{2\pi K\tilde{T}} \right)^{3/2} \exp \left[-\frac{m^s}{2K\tilde{T}} (\mathbf{v} - \tilde{\mathbf{u}})^2 \right] \quad s = 1, \dots, 4, \quad (6)$$

with seven disposable scalar parameters, provided by $\tilde{n}^s, \tilde{\mathbf{u}}, \tilde{T}$, bound together by the mass action law

$$\frac{\tilde{n}^1 \tilde{n}^2}{\tilde{n}^3 \tilde{n}^4} = \left(\frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \exp \left(\frac{\Delta E}{K\tilde{T}} \right) \quad (7)$$

so that, unlike previous models, this collision operator drives the gas toward a full, mechanical and chemical, equilibrium as it is appropriate when the two processes proceed at the same pace. In Eq. (5) the factor ν_s is the inverse of the s th relaxation time, possibly depending on macroscopic fields but independent of \mathbf{v} . Here and below macroscopic parameters for each species are defined in the usual way, and global observable fields (including mass density ρ , viscosity tensor \mathbf{p} , and heat flux \mathbf{q}) are expressed in terms of single component parameters by

$$\begin{aligned} n &= \sum_{s=1}^4 n^s, \quad \rho = \sum_{s=1}^4 m^s n^s, \quad \mathbf{u} = \frac{1}{\rho} \sum_{s=1}^4 m^s n^s \mathbf{u}^s, \\ nKT &= \sum_{s=1}^4 n^s KT^s + \frac{1}{3} \sum_{s=1}^4 \rho^s (u_k^s u_k^s - u_k u_k), \\ p_{ij} &= \sum_{s=1}^4 p_{ij}^s + \sum_{s=1}^4 \rho^s \left[(u_i^s u_j^s - u_i u_j) - \frac{1}{3} \delta_{ij} (u_k^s u_k^s - u_k u_k) \right], \\ q_i &= \sum_{s=1}^4 q_i^s + \sum_{s=1}^4 p_{ij}^s (u_j^s - u_j) + \frac{5}{2} \sum_{s=1}^4 n^s KT^s (u_i^s - u_i) \\ &\quad + \frac{1}{2} \sum_{s=1}^4 \rho^s (u_k^s - u_k) (u_k^s - u_k) (u_i^s - u_i). \end{aligned} \quad (8)$$

The auxiliary fields $\tilde{n}^s, \tilde{\mathbf{u}}, \tilde{T}$ in Eqs. (6) and (7) are determined in terms of the actual fields n^s, \mathbf{u}^s, T^s by requiring that the present approximation and the actual Boltzmann description share the same collision invariants. Referring the interested reader to [17,18] for details and discussion, this leads to the algebraic system

$$\tilde{n}^s = n^s + \lambda^s \frac{\nu_1}{\nu_s} (\tilde{n}^1 - n^1), \quad s = 2, 3, 4,$$

$$\tilde{\mathbf{u}} = \sum_{s=1}^4 \nu_s m^s n^s \mathbf{u}^s \bigg/ \sum_{s=1}^4 \nu_s m^s n^s,$$

$$\tilde{T} = \frac{\left\{ \sum_{s=1}^4 \nu_s n^s \left[\frac{1}{2} \nu_s m^s [(u^s)^2 - \tilde{u}^2] + \frac{3}{2} K T^s \right] + \nu_1 \Delta E (\tilde{n}^1 - n^1) \right\}}{\left(\frac{3}{2} K \sum_{s=1}^4 \nu_s n^s \right)}$$

$$= \tilde{T}(\tilde{n}^1) \quad (9)$$

so that $\tilde{\mathbf{u}}$ follows directly from the actual fields, and all other parameters are cast in terms of the single variable \tilde{n}^1 . The latter is determined finally by the mass action law, given by Eq. (7), which can be written as a transcendental equation

$$\frac{\nu_3 \nu_4 \tilde{n}^1 [\nu_2 n^2 + \nu_1 (\tilde{n}^1 - n^1)]}{\nu_2 [\nu_3 n^3 - \nu_1 (\tilde{n}^1 - n^1)] [\nu_4 n^4 - \nu_1 (\tilde{n}^1 - n^1)]} \exp\left(-\frac{\Delta E}{K \tilde{T}(\tilde{n}^1)}\right) = \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2}, \quad (10)$$

with $\tilde{T}(\tilde{n}^1)$ defined by Eq. (9). It can be proved finally by monotonicity arguments that Eq. (10) admits a unique physical solution, which guarantees well posedness for the proposed algorithm, working then properly without any restriction on collision model and physical regime.

Conserved quantities coincide with those of the Boltzmann collision process and may be chosen as three combinations of number densities such as $n^1 + n^3$, $n^1 + n^4$, $n^2 + n^4$, the three components of the mass velocity \mathbf{u} , and the total internal (thermal+chemical) energy $\frac{3}{2} n K T + \sum_{s=1}^4 E^s n^s$. Correspondingly, the ‘‘exact’’ set of seven scalar nonclosed macroscopic conservation equations

$$\frac{\partial}{\partial t} (n^s + n^r) + \frac{\partial}{\partial \mathbf{x}} \cdot (n^s \mathbf{u}^s + n^r \mathbf{u}^r) = 0$$

$$(s, r) = (1, 3), (1, 4), (2, 4),$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{P}) = \mathbf{0},$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho u^2 + \frac{3}{2} n K T + \sum_{s=1}^4 E^s n^s \right) + \frac{\partial}{\partial \mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho u^2 + \frac{3}{2} n K T + \sum_{s=1}^4 E^s n^s \right) \mathbf{u} + \mathbf{P} \cdot \mathbf{u} + \mathbf{q} + \sum_{s=1}^4 E^s n^s (\mathbf{u}^s - \mathbf{u}) \right] = 0, \quad (11)$$

where $\mathbf{P} = n K T \mathbf{I} + \mathbf{p}$ is the pressure tensor, is recovered. In addition, collision equilibria for this model also coincide with the correct ones and are provided by the seven parameter family of Maxwellians satisfying the mass action law, as given by Eqs. (2) and (3). Finally, an outstanding feature of the present relaxation model is that it allows for an explicit analytical proof of an H theorem [17], a result that was missing in previous reactive BGK models, the H functional being again given by the same as for the Boltzmann equations, namely, by Eq. (4). We only point out here that a crucial role

in the proof is played by Eq. (7), meaning that, like for an inert mixture, the attractor is itself, by definition, a collision equilibrium, from which the Boltzmann inequality easily follows.

Concerning the most convenient choice of the inverse relaxation times ν_s , which is a problem of minor relevance for the developments in this paper (though affecting crucially the final result), we refer once more to the quoted literature, in particular to [17]. With the strategy of reproducing the actual average number of collisions (namely, the total averaged loss terms) taking place for each species, and for given trends (for instance, powerlike [26]) of microscopic collision frequencies over their supports, such macroscopic parameters can be handled analytically. We report here, just for illustration, the simplest closed form expression, relevant to Maxwell-like assumption on elastic and exothermic differential cross sections

$$\nu_1 = \sum_{s=1}^4 \nu_{1s} n^s + \left(\frac{\mu^{34}}{\mu^{12}}\right)^{3/2} \exp\left(-\frac{\Delta E}{K T}\right) \nu_{34}^{12} n^2,$$

$$\nu_2 = \sum_{s=1}^4 \nu_{2s} n^s + \left(\frac{\mu^{34}}{\mu^{12}}\right)^{3/2} \exp\left(-\frac{\Delta E}{K T}\right) \nu_{34}^{12} n^1,$$

$$\nu_3 = \sum_{s=1}^4 \nu_{3s} n^s + \nu_{34}^{12} n^4,$$

$$\nu_4 = \sum_{s=1}^4 \nu_{4s} n^s + \nu_{34}^{12} n^3, \quad (12)$$

where ν_{rs} and ν_{34}^{12} are given constants. They show dependence on number densities and temperature, and count elastic and reactive interactions with equal weight in making up the macroscopic collision frequencies ν_s as it is appropriate when mechanical and chemical processes are equally fast.

III. HYDRODYNAMIC REGIME

Equations (5) may be scaled, measuring all quantities in terms of some typical values. Using macroscopic scales for space and time variables and measuring microscopic parameters in units of typical values leads to equations which look exactly the same as Eq. (5) if the same symbol is retained for dimensionless variables, with only the appearance of the Knudsen number ε , ratio of the microscopic to the macroscopic time scales, as

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \frac{\partial f^s}{\partial \mathbf{x}} = \frac{1}{\varepsilon} \nu_s (\mathcal{M}_s - f^s) \quad s = 1, \dots, 4, \quad (13)$$

where the small parameter ε tends to zero in the continuum limit we are interested in. We shall perform a formal Chapman-Enskog asymptotic analysis to first-order accuracy, in order to achieve a Navier-Stokes hydrodynamic closure of the conservation laws given by Eqs. (11). To this end, the distribution functions f^s are expanded as

$$f^s = f^{s(0)} + \varepsilon f^{s(1)}, \quad (14)$$

and consequently similar expansions hold for n^s , \mathbf{u}^s , and T^s . However, hydrodynamic variables must remain unexpanded [27], namely,

$$n^s + n^r = n^{s(0)} + n^{r(0)} \quad (s, r) = (1, 3), (1, 4), (2, 4),$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{s=1}^4 m^s n^{s(0)} \mathbf{u}^{s(0)},$$

$$\frac{3}{2} n T + \sum_{s=1}^4 E^s n^s = \frac{3}{2} n T^{(0)} + \sum_{s=1}^4 E^s n^{s(0)} \quad (15)$$

(with $n = \sum_{s=1}^4 n^{s(0)}$ and $\rho = \sum_{s=1}^4 m^s n^{s(0)}$ not expanded either), yielding the constraints

$$n^{1(1)} = n^{2(1)} = -n^{3(1)} = -n^{4(1)} = \frac{3n}{2\Delta E} T^{(1)},$$

$$\sum_{s=1}^4 m^s n^{s(0)} \mathbf{u}^{s(1)} + \sum_{s=1}^4 m^s n^{s(1)} \mathbf{u}^{s(0)} = \mathbf{0}. \quad (16)$$

Notice that, contrary to classical (nonreactive) gas dynamics, temperature is not an hydrodynamic field so that it must also be expanded as $T = T^{(0)} + \varepsilon T^{(1)}$. These expansions induce of course similar expansions for all variables, in particular for the auxiliary fields and for the Maxwellians \mathcal{M}_s . The macroscopic collision frequencies ν_s , depending on the densities n^s , must be expanded as well. Equating finally equal powers of ε in Eq. (13) yields to leading order

$$\mathcal{M}_s^{(0)}(\mathbf{v}) - f^{s(0)}(\mathbf{v}) = 0, \quad (17)$$

and to the next order

$$\nu_s^{(0)} [\mathcal{M}_s^{(1)}(\mathbf{v}) - f^{s(1)}(\mathbf{v})] = \frac{\partial_0 f^{s(0)}}{\partial t} + \mathbf{v} \cdot \frac{\partial f^{s(0)}}{\partial \mathbf{x}}, \quad (18)$$

where $\partial_0 / \partial t$ is the first term of a formal expansion of the time derivative operator, to be considered as an unknown of the problem.

These are uneasy highly nonlinear integrofunctional equations for the unknowns $f^{s(i)}$, since their integral moments are needed in the definition of the parameters determining the auxiliary Maxwellians $\mathcal{M}_s^{(i)}$. However, Eqs. (17) yield, in cascade, $n^{s(0)} = \tilde{n}^{s(0)}$, $\mathbf{u}^{s(0)} = \tilde{\mathbf{u}}^{s(0)}$, $T^{s(0)} = \tilde{T}^{s(0)}$, then the zero-order mass action law

$$\frac{n^{1(0)} n^{2(0)}}{n^{3(0)} n^{4(0)}} = \left(\frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \exp\left(\frac{\Delta E}{T^{(0)}} \right). \quad (19)$$

Notice that all species share, to leading order, the same drift velocity, equal thus to the global mass velocity \mathbf{u} , and the same temperature, equal to the leading term of the global temperature T . In conclusion we have

$$f^{s(0)}(\mathbf{v}) = n^{s(0)} \left(\frac{m^s}{2\pi T^{(0)}} \right)^{3/2} \exp\left[-\frac{m^s}{2T^{(0)}} (\mathbf{v} - \mathbf{u})^2 \right], \quad (20)$$

for $s=1, \dots, 4$, with seven free parameters since the $n^{s(0)}$ and $T^{(0)}$ must be bound together by Eq. (19). Equations (20) yield immediately $p_{ij}^{s(0)} = 0$ and $q_i^{s(0)} = 0$ for all s , from which also $p_{ij}^{(0)} = 0$ and $q_i^{(0)} = 0$ for the leading terms of viscosity tensor and heat flux.

Before going on to the next step, we can select as unknowns for the sought Navier-Stokes-type equations the seven scalar variables $n^{s(0)}$, $s=1, \dots, 4$, and \mathbf{u} , and express $T^{(0)}$, wherever needed, by means of Eq. (19). Conservation equations may be rewritten as

$$\begin{aligned} & \frac{\partial}{\partial t} (n^{s(0)} + n^{r(0)}) + \frac{\partial}{\partial \mathbf{x}} \cdot [(n^{s(0)} + n^{r(0)}) \mathbf{u}] \\ & + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot (n^{s(0)} \mathbf{u}^{s(1)} + n^{r(0)} \mathbf{u}^{r(1)}) = 0 \\ & (s, r) = (1, 3), (1, 4), (2, 4), \end{aligned}$$

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho \mathbf{u}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \frac{\partial}{\partial \mathbf{x}} (n T^{(0)}) \\ & + \varepsilon \frac{\partial}{\partial \mathbf{x}} (n T^{(1)}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{p}^{(1)} = \mathbf{0}, \end{aligned}$$

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\frac{1}{2} \rho u^2 + \frac{3}{2} n T^{(0)} + \sum_{s=1}^4 E^s n^{s(0)} \right) \\ & + \frac{\partial}{\partial \mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho u^2 + \frac{5}{2} n T^{(0)} + \sum_{s=1}^4 E^s n^{s(0)} \right) \mathbf{u} \right] \\ & + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot (n T^{(1)} \mathbf{u}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} (\mathbf{p}^{(1)} \cdot \mathbf{u}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{q}^{(1)} \\ & + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot \left(\sum_{s=1}^4 E^s n^{s(0)} \mathbf{u}^{s(1)} \right) = 0, \quad (21) \end{aligned}$$

and their closure is achieved if we are able to determine, resorting to Eq. (18), constitutive equations for the quantities $\mathbf{u}^{s(1)}$, $T^{(1)}$, $p_{ij}^{(1)}$, and $q_i^{(1)}$, for which we have further

$$\begin{aligned} n T^{(1)} &= \sum_{s=1}^4 n^{s(0)} T^{s(1)}, \quad p_{ij}^{(1)} = \sum_{s=1}^4 p_{ij}^{s(1)}, \\ q_i^{(1)} &= \sum_{s=1}^4 q_i^{s(1)} + \frac{5}{2} T^{(0)} \sum_{s=1}^4 n^{s(0)} u_i^{s(1)}. \quad (22) \end{aligned}$$

IV. FIRST-ORDER CORRECTION

Lengthy but standard manipulations allow to evaluate the time and space derivatives of $f^{s(0)}$ and to express $\mathcal{M}_s^{(1)}$ as the derivative of \mathcal{M}_s with respect to ε at $\varepsilon=0$; in this way we obtain a formal solution of Eq. (18) as

$$f^{s(1)} = f^{s(0)} \left\{ \frac{1}{n^{s(0)}} \tilde{n}^{s(1)} + \frac{m^s}{T^{(0)}} \tilde{\mathbf{u}}^{(1)} \cdot (\mathbf{v} - \mathbf{u}) + \frac{1}{T^{(0)}} \tilde{T}^{(1)} \left[\frac{m^s}{2T^{(0)}} (\mathbf{v} - \mathbf{u})^2 - \frac{3}{2} \right] \right\} - \frac{1}{\nu_s^{(0)}} f^{s(0)} \left\{ \frac{1}{n^{s(0)}} \frac{\partial_0 n^{s(0)}}{\partial t} + \frac{m^s}{T^{(0)}} \frac{\partial_0 \mathbf{u}}{\partial t} \cdot (\mathbf{v} - \mathbf{u}) \right. \\ \left. + \frac{1}{T^{(0)}} \frac{\partial_0 T^{(0)}}{\partial t} \left[\frac{m^s}{2T^{(0)}} (\mathbf{v} - \mathbf{u})^2 - \frac{3}{2} \right] \right\} - \frac{1}{\nu_s^{(0)}} f^{s(0)} \left\{ \frac{1}{n^{s(0)}} \frac{\partial n^{s(0)}}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{m^s}{T^{(0)}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}} : \mathbf{v} \otimes (\mathbf{v} - \mathbf{u}) + \frac{1}{T^{(0)}} \frac{\partial T^{(0)}}{\partial \mathbf{x}} \cdot \left[\frac{m^s}{2T^{(0)}} (\mathbf{v} - \mathbf{u})^2 - \frac{3}{2} \right] \mathbf{v} \right\}, \quad (23)$$

where $\tilde{n}^{s(1)}$, $\tilde{\mathbf{u}}^{(1)}$, $\tilde{T}^{(1)}$ are the first-order corrections of the auxiliary fields as obtained by the asymptotic expansion of the results following from Eqs. (9) and (10). After patient manipulations, the first row in Eq. (9) yields

$$\tilde{n}^{s(1)} = n^{s(1)} + \frac{\lambda^s J_1}{\nu_s^{(0)}} \quad s = 2, 3, 4, \quad J_1 = \nu_1^{(0)} (\tilde{n}^{1(1)} - n^{1(1)}), \quad (24)$$

which gives all auxiliary density corrections in terms of actual moments and of J_1 . The second row in Eq. (9) yields then

$$\tilde{\mathbf{u}}^{(1)} = \left[\sum_{s=1}^4 \nu_s^{(0)} m^s n^{s(0)} \right]^{-1} \left[\sum_{s=1}^4 \nu_s^{(0)} m^s n^{s(0)} \mathbf{u}^{s(1)} \right], \quad (25)$$

expressing auxiliary velocity correction in terms of actual moments only. The third row in Eq. (9) leads to

$$\tilde{T}^{(1)} = \left[\sum_{s=1}^4 \nu_s^{(0)} n^{s(0)} \right]^{-1} \left[\sum_{s=1}^4 \nu_s^{(0)} n^{s(0)} T^{s(1)} + \frac{2}{3} \Delta E J_1 \right], \quad (26)$$

and finally Eq. (10) yields, after some algebra,

$$J_1 = - \left[\sum_{s=1}^4 \frac{n^{1(1)}}{n^{s(0)}} + \frac{\Delta E}{T^{(0)}} \frac{\sum_{s=1}^4 \nu_s^{(0)} n^{s(0)} T^{s(1)}}{\sum_{s=1}^4 \nu_s^{(0)} n^{s(0)} T^{(0)}} \right] \\ \times \left[\sum_{s=1}^4 \frac{1}{\nu_s^{(0)} n^{s(0)}} + \frac{2}{3} \frac{(\Delta E/T^{(0)})^2}{\sum_{s=1}^4 \nu_s^{(0)} n^{s(0)}} \right]^{-1}. \quad (27)$$

In this way the distribution functions (23) are cast in terms of the actual moments $n^{s(1)}$, $\mathbf{u}^{s(1)}$, $T^{s(1)}$ and of the operators $\partial_0/\partial t$, all still unknown. In order to make their knowledge effective, and not only formal, we need to recompute the moments by means of

$$\int f^{s(1)}(\mathbf{v}) d\mathbf{v} = n^{s(1)}, \quad \int \mathbf{v} f^{s(1)}(\mathbf{v}) d\mathbf{v} = n^{s(1)} \mathbf{u} + n^{s(0)} \mathbf{u}^{s(1)},$$

$$\int (\mathbf{v} - \mathbf{u})^2 f^{s(1)}(\mathbf{v}) d\mathbf{v} = \frac{3}{m^s} (n^{s(1)} T^{(0)} + n^{s(0)} T^{s(1)}), \quad (28)$$

applying the compatibility conditions following from the previously established constraints, in order to get rid of the unknowns $\partial_0 n^{s(0)}/\partial t$ and $\partial_0 \mathbf{u}/\partial t$, whereas $\partial_0 T^{(0)}/\partial t$ is provided by the zero-order mass action law as

$$\frac{1}{T^{(0)}} \frac{\partial_0 T^{(0)}}{\partial t} = - \frac{T^{(0)}}{\Delta E} \sum_{s=1}^4 \frac{\lambda^s}{n^{s(0)}} \frac{\partial_0 n^{s(0)}}{\partial t}. \quad (29)$$

Skipping technical details, density fields provide the compatibility conditions

$$\frac{\partial_0 n^{s(0)}}{\partial t} = - \frac{\partial}{\partial \mathbf{x}} \cdot (n^{s(0)} \mathbf{u}) + \lambda^s J_1 \quad s = 1, \dots, 4. \quad (30)$$

Velocity fields yield the compatibility conditions

$$\frac{\partial_0 \mathbf{u}}{\partial t} = - \mathbf{u} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{x}} - \frac{1}{\rho} \frac{\partial}{\partial \mathbf{x}} (n T^{(0)}) \quad (31)$$

and the algebraic equations

$$\sum_{r=1}^4 \phi^{sr(0)} \mathbf{u}^{r(1)} = \frac{\partial}{\partial \mathbf{x}} (n^{s(0)} T^{(0)}) - \frac{\rho^{s(0)}}{\rho} \frac{\partial}{\partial \mathbf{x}} (n T^{(0)}), \quad s = 1, \dots, 4, \quad (32)$$

where the singular matrix $\phi^{sr(0)}$ has the form

$$\phi^{sr(0)} = \nu_s^{(0)} \rho^{s(0)} \left(\frac{\nu_r^{(0)} \rho^{r(0)}}{\sum_{j=1}^4 \nu_j^{(0)} \rho^{j(0)}} - \delta_{sr} \right), \quad (33)$$

with

$$\sum_{s=1}^4 \phi^{sr(0)} = 0 \quad r = 1, \dots, 4, \quad \sum_{s=1}^4 \rho^{s(0)} \mathbf{u}^{s(1)} = \mathbf{0}, \quad (34)$$

so that the algebraic Eqs. (32) are indeed uniquely solvable. This set of equations has the same structure as those arising when the Chapman-Enskog algorithm is applied to the either Grad 13-moment approximation of the reactive Boltzmann equations [25], or to the BGK model equations in the chemically neutral version [10]. It is remarkable however that the present matrix accounts for both mechanical and chemical encounters via the inverse relaxation times $\nu_s^{(0)}$, whereas in the slow reactive frame only the mechanical collision frequencies were involved. In any case the solution, *mutatis*

mutandis, goes through the same steps of either [10] or [25] and may be cast as

$$\mathbf{u}^{s(1)} = - \sum_{r=1}^4 L^{sr(0)} \frac{1}{\rho^{s(0)} \rho^{r(0)}} \frac{\partial}{\partial \mathbf{x}} (n^{r(0)} T^{(0)}) \quad (35)$$

where $L^{sr(0)}$ is a suitable (singular) matrix, depending on the densities $n^{s(0)}$, which can be proved to be symmetric [10], reproducing thus the Onsager relations [28].

Finally, temperature fields recomputed from Eq. (23) yield a set of linear algebraic equations for the $T^{s(1)}$ with matrix coefficients

$$\psi^{sr(0)} = \nu_s^{(0)} n^{s(0)} \left(\frac{\nu_r^{(0)} n^{r(0)}}{4} - \delta_{sr} \right), \quad (36)$$

$$\left(\sum_{j=1}^4 \nu_j^{(0)} n^{j(0)} \right)$$

which make up again a singular matrix of the same structure as Eq. (33). Now a compatibility condition must be applied to the inhomogeneous terms of the algebraic system. Taking into account that Eq. (19) implies

$$\frac{1}{T^{(0)}} \frac{\partial T^{(0)}}{\partial x_i} = - \frac{T^{(0)}}{\Delta E} \sum_{s=1}^4 \frac{\lambda^s}{n^{s(0)}} \frac{\partial n^{s(0)}}{\partial x_i}, \quad (37)$$

a little algebra yields

$$J_1 = \left(\frac{n T^{(0)}}{\Delta E} \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{u} \right) \left[1 + \frac{3}{2} n \left(\frac{T^{(0)}}{\Delta E} \right)^2 \sum_{s=1}^4 \frac{1}{n^{s(0)}} \right]^{-1}. \quad (38)$$

Now, starting from

$$n T^{(1)} = \frac{1}{3} \sum_{s=1}^4 m^s \int (\mathbf{v} - \mathbf{u})^2 f^{s(1)}(\mathbf{v}) d\mathbf{v}, \quad (39)$$

it is matter of some simple manipulations to show that $T^{(1)}$ can be cast in terms of zero-order moments and J_1 only so that, on using Eq. (38), we are led to the explicit expression

$$T^{(1)} = - \frac{2}{3} T^{(0)} \frac{\frac{1}{n} \sum_{s=1}^4 \frac{n^{s(0)}}{\nu_s^{(0)}} + \frac{3}{2} n \left(\frac{T^{(0)}}{\Delta E} \right)^2 \sum_{s=1}^4 \frac{1}{\nu_s^{(0)} n^{s(0)}}}{\left[1 + \frac{3}{2} n \left(\frac{T^{(0)}}{\Delta E} \right)^2 \sum_{s=1}^4 \frac{1}{n^{s(0)}} \right]^2} \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{u}. \quad (40)$$

It is interesting to remark that this correction is specific of reactive mixtures [29] and is not present in any inert problem.

In principle, the procedure is so completed since now we could solve uniquely the algebraic equations for $T^{s(1)}$ and obtain all first-order corrections, actual and fictitious, in terms of the chosen hydrodynamic variables and their gradients so that the distribution functions (23) would be fully explicit. We shall not do that since it suffices to compute the viscous stress $p_{ij}^{(1)}$ and the heat flux $q_i^{(1)}$ by suitable integration of the distribution functions in order to close the macroscopic Eqs. (21) and to achieve the sought Navier-Stokes equations.

For that purpose we have

$$P_{ij}^{s(1)} = m^s \int_{\mathbb{R}^3} (v_i - u_i)(v_j - u_j) f^{s(1)}(\mathbf{v}) d\mathbf{v},$$

$$p_{ij}^{s(1)} = P_{ij}^{s(1)} - \delta_{ij} \frac{1}{3} \text{tr} \mathbf{P}^{s(1)} \quad (41)$$

and

$$q_i^{s(1)} = - \frac{5}{2} T^{(0)} n^{s(0)} u_i^{s(1)} + \frac{1}{2} m^s \int_{\mathbb{R}^3} (v_i - u_i)(\mathbf{v} - \mathbf{u})^2 f^{s(1)} d\mathbf{v} \quad (42)$$

to be used then in Eqs. (22). When computing $P_{ij}^{s(1)}$, it is not difficult to check that the addends of $f^{s(1)}$ involving the first curly brackets of Eq. (23) yield a tensor proportional to the identity, which contributes nothing to the deviatoric part $p_{ij}^{s(1)}$, and the same occurs to the addends from the second curly brackets, involving the $\partial_0/\partial t$ operator. For the third curly brackets, involving spatial gradients, the same feature is in order for the gradients of $n^{s(0)}$ and $T^{(0)}$, whereas the rate of strain tensor contributes a term

$$- \frac{n^{s(0)} T^{(0)}}{\nu_s^{(0)}} \left[\delta_{ij} \left(2 \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{u} \right) + (1 - \delta_{ij}) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right], \quad (43)$$

where the square bracket is the sum of $\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}$ and of an isotropic tensor. Going on and computing $p_{ij}^{s(1)}$ and $q_i^{(1)}$, one ends up with

$$p_{ij}^{(1)} = - T^{(0)} \sum_{s=1}^4 \frac{n^{s(0)}}{\nu_s^{(0)}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{u} \delta_{ij} \right). \quad (44)$$

This Newtonian constitutive equation corresponds to a viscosity coefficient

$$\mu = T^{(0)} \sum_{s=1}^4 \frac{n^{s(0)}}{\nu_s^{(0)}}, \quad (45)$$

formally the same obtained in [10] from the BGK equations for a chemically neutral gas mixture. An expression of the same type was obtained for the slow reactive case in [25] by the Grad method but with a different viscosity coefficient that was provided there by a formal inversion of suitable matrices. Passing to Eq. (42), we may split $f^{s(1)}$ in three different addends as before and evaluate separately the relevant contributions. Skipping details and putting together all terms there results

$$q_i^{s(1)} = - \frac{5}{2} \frac{n^{s(0)} T^{(0)}}{\nu_s^{(0)}} \left[\frac{\partial_0 u_i}{\partial t} + \mathbf{u} \cdot \frac{\partial u_i}{\partial \mathbf{x}} + \frac{1}{\rho^{s(0)}} \frac{\partial}{\partial x_i} (n^{s(0)} T^{(0)}) \right]$$

$$- \frac{5}{2} \frac{n^{s(0)} T^{(0)}}{m^s \nu_s^{(0)}} \frac{\partial T^{(0)}}{\partial x_i} + \frac{5}{2} T^{(0)} n^{s(0)} (\tilde{u}_i^{(1)} - u_i^{s(1)}), \quad (46)$$

and upon using Eq. (25) for $\tilde{u}_i^{(1)}$ and Eqs. (31) and (32) for the square bracket, we end up simply with

$$q_i^{s(1)} = -\frac{5}{2}T^{(0)} \frac{n^{s(0)}}{m^s \nu_s^{(0)}} \frac{\partial T^{(0)}}{\partial x_i}. \quad (47)$$

In conclusion, from the last of Eqs. (22),

$$q_i^{(1)} = -\frac{5}{2}T^{(0)} \sum_{s=1}^4 \frac{n^{s(0)}}{m^s \nu_s^{(0)}} \frac{\partial T^{(0)}}{\partial x_i} + \frac{5}{2}T^{(0)} \sum_{s=1}^4 n^{s(0)} u_i^{s(1)}, \quad (48)$$

a Fourier conduction law with a thermal conductivity

$$\lambda = \frac{5}{2}T^{(0)} \sum_{s=1}^4 \frac{n^{s(0)}}{m^s \nu_s^{(0)}}. \quad (49)$$

Again this result coincides formally with the corresponding one for the same BGK strategy applied to a nonreactive mix-

ture [10], and reproduces the structure of heat flux for the slow reactive case as obtained by the Grad method [25], only with a different conductivity, which is explicitly given here, whereas requires the inversion of certain matrices there.

V. COMMENTS AND CONCLUSIONS

Summarizing our results, hydrodynamic equations of Navier-Stokes type for the present relaxation model of the chemical reaction described by Eq. (1) are provided by Eqs. (21), a set of seven partial differential equations for the seven scalar unknowns $n^{s(0)}$ and \mathbf{u} , coupled to the transcendental algebraic Eq. (19) for $T^{(0)}$, and to the proper constitutive equations, namely Eqs. (35) for $u_i^{s(1)}$, Eq. (40) for $T^{(1)}$, Eq. (44) for $p_{ij}^{(1)}$, and Eq. (48) for $q_i^{(1)}$. All together, they read as

$$\frac{\partial}{\partial t} (n^{s(0)} + n^{r(0)}) + \frac{\partial}{\partial \mathbf{x}} \cdot [(n^{s(0)} + n^{r(0)})\mathbf{u}] + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot (n^{s(0)}\mathbf{u}^{s(1)} + n^{r(0)}\mathbf{u}^{r(1)}) = 0,$$

$$(s, r) = (1, 3), (1, 4), (2, 4),$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \frac{\partial}{\partial \mathbf{x}} (nT^{(0)}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} (nT^{(1)}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{p}^{(1)} = \mathbf{0},$$

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{1}{2} \rho u^2 + \frac{3}{2} nT^{(0)} + \sum_{s=1}^4 E^s n^{s(0)} \right) + \frac{\partial}{\partial \mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho u^2 + \frac{5}{2} nT^{(0)} + \sum_{s=1}^4 E^s n^{s(0)} \right) \mathbf{u} \right] \\ + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot (nT^{(1)}\mathbf{u}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} (\mathbf{p}^{(1)} \cdot \mathbf{u}) + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{q}^{(1)} + \varepsilon \frac{\partial}{\partial \mathbf{x}} \cdot \left(\sum_{s=1}^4 E^s n^{s(0)} \mathbf{u}^{s(1)} \right) = 0, \end{aligned}$$

$$\frac{n^{1(0)} n^{2(0)}}{n^{3(0)} n^{4(0)}} = \left(\frac{\mu^{12}}{\mu^{34}} \right)^{3/2} \exp \left(\frac{\Delta E}{T^{(0)}} \right),$$

$$\mathbf{u}^{s(1)} = - \sum_{r=1}^4 L^{sr(0)} \frac{1}{\rho^{s(0)} \rho^{r(0)}} \frac{\partial}{\partial \mathbf{x}} (n^{r(0)} T^{(0)}),$$

$$T^{(1)} = -\frac{2}{3} T^{(0)} \frac{\frac{1}{n} \sum_{s=1}^4 \frac{n^{s(0)}}{\nu_s^{(0)}} + \frac{3}{2} n \left(\frac{T^{(0)}}{\Delta E} \right)^2 \sum_{s=1}^4 \frac{1}{\nu_s^{(0)} n^{s(0)}}}{\left[1 + \frac{3}{2} n \left(\frac{T^{(0)}}{\Delta E} \right)^2 \sum_{s=1}^4 \frac{1}{n^{s(0)}} \right]^2} \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{u},$$

$$p_{ij}^{(1)} = -T^{(0)} \sum_{s=1}^4 \frac{n^{s(0)}}{\nu_s^{(0)}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{u} \delta_{ij} \right),$$

$$q_i^{(1)} = -\frac{5}{2} T^{(0)} \sum_{s=1}^4 \frac{n^{s(0)}}{m^s \nu_s^{(0)}} \frac{\partial T^{(0)}}{\partial x_i} + \frac{5}{2} T^{(0)} \sum_{s=1}^4 n^{s(0)} u_i^{s(1)}. \quad (50)$$

Euler equations correspond to the limiting case $\varepsilon=0$.

The present BGK asymptotic limit differs substantially from the BGK asymptotic limit that would be in order if the chemical reaction were switched off, that was thoroughly derived and discussed in [10], as well as from the Grad asymptotic limit for a slowly reactive mixture, worked out in [25]. In those cases in fact the kernel of the collision operator is eight dimensional, and all densities, as well as the temperature, are hydrodynamic variables so that Navier-Stokes equations are made up by eight partial differential equations, including continuity equations for each species. The slow reactive case includes an additional chemical source term, but transport coefficients are determined only by mechanical collision parameters. The present reactive Navier-Stokes equations are made up by seven partial differential equations for seven unknowns, with only three pairwise coupled continuity equations for the species, and with temperature following from the actual unknowns by means of the mass action law, indicating an evolution close to the chemical equilibrium. Therefore one should look at Eqs. (50) in a different way since all temperature gradients in both differential and constitutive equations must be restated in terms of density gradients, resorting to Eq. (37). From a different point of view, one could deal with the eight usual observable fields and consider these Navier-Stokes equations as a closed set of differential-algebraic equations. Transport coefficients underlying the constitutive equations for diffusion velocities, viscous stress, and heat flux are formally, *mutatis mutandis*, the classical ones from the nonreactive Boltzmann equations [22], but the matrix $L^{sr(0)}$, the viscosity coefficient μ , and the thermal conductivity λ are built up in terms of the macroscopic collision frequencies $\nu_s^{(0)}$, which account for not only elastic scattering, but also reactive collisions since

$$\nu_1^{(0)} = \sum_{s=1}^4 \nu_{1s} n^{s(0)} + \left(\frac{\mu^{34}}{\mu^{12}} \right)^{3/2} \exp\left(-\frac{\Delta E}{T^{(0)}}\right) \nu_{34}^{12} n^{2(0)},$$

$$\nu_2^{(0)} = \sum_{s=1}^4 \nu_{2s} n^{s(0)} + \left(\frac{\mu^{34}}{\mu^{12}} \right)^{3/2} \exp\left(-\frac{\Delta E}{T^{(0)}}\right) \nu_{34}^{12} n^{1(0)},$$

$$\nu_3^{(0)} = \sum_{s=1}^4 \nu_{3s} n^{s(0)} + \nu_{34}^{12} n^{4(0)},$$

$$\nu_4^{(0)} = \sum_{s=1}^4 \nu_{4s} n^{s(0)} + \nu_{34}^{12} n^{3(0)} \quad (51)$$

so that chemical reactions do affect the hydrodynamic closure and the transport coefficients themselves. Notice that, for slow chemistry, reactive collision parameters [namely, in the approximation introduced by Eqs. (12), the microscopic collision frequency ν_{34}^{12}] would be one order of magnitude smaller (in units of ε) than the mechanical ones so that the leading terms $\nu_s^{(0)}$ would include only elastic scattering, leading back to a scenario closer to [25]. This indicates that neglecting effects of the chemical reaction on diffusion, viscosity, and conductivity coefficients can be regarded as a reasonable approximation when the reaction is slow but would not be consistent when the reaction is fast. On the other hand, this is in agreement with physical expectation and is confirmed also by other theoretical approaches, such as for instance those of Refs. [30,31]. In these papers explicit reaction-dependent expressions for transport coefficients have been derived either by a truncated Sonine polynomial expansion for a binary mixture (in the former) or by approximating some collision integrals in terms of suitable “input” functions (in the latter). The effects of chemical reactions are also accounted for, in agreement with heuristic and thermodynamical considerations, by an additional reactive scalar pressure $nT^{(1)}$ [29], involving the divergence of mass velocity, instead of an additional chemical source term of algebraic type that would be typical for slow reactions [25]. The present analysis shows how this experimentally observed chemical pressure comes into the picture by a mathematical requirement since, in the present fast reactive frame, the gas temperature is not a conserved quantity. In fact, only the total energy, involving a chemical contribution in addition to the thermal one, is conserved by the dominant operator driving the overall evolution, and therefore also a first-order correction to the temperature must be considered in the asymptotic scheme and evaluated in terms of the chosen macroscopic fields. Clearly, if the reaction were switched off, we would be led back to the constitutive equations of the inert BGK hydrodynamic limit [10]; in this respect, as typical in kinetic theory, viscosity, and conductivity are expressed in closed form if derived from a BGK level description, contrary to the more complicated implicit expressions obtained from the Boltzmann or Grad level [25].

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