

Regularization of Grad's 13 moment equations: Derivation and linear analysis

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A new closure for Grad's 13 moment equations is presented that adds terms of Super-Burnett order to the balances of pressure deviator and heat flux vector. The additional terms are derived from equations for higher moments by means of the distribution function for 13 moments. The resulting system of equations contains the Burnett and Super-Burnett equations when expanded in a series in the Knudsen number. However, other than the Burnett and Super-Burnett equations, the new set of equations is linearly stable for *all* wavelengths and frequencies. Dispersion relation and damping for the new equations agree better with experimental data than those for the Navier–Stokes–Fourier equations, or the original 13 moments system. The new equations also allow the description of Knudsen boundary layers. © 2003 American Institute of Physics. [DOI: 10.1063/1.1597472]

I. INTRODUCTION

Processes in rarefied gases are well described by the Boltzmann equation.^{1,2} The numerical solution of the Boltzmann equation, either directly³ or via the direct simulation Monte Carlo (DSMC) method,⁴ is very time expensive in certain regimes, particularly at low Mach numbers in the transition regime.⁵ Since this regime is important for the simulation of microscale flows, e.g., in microelectromechanical systems, there is a strong desire for accurate models which allow the calculation of processes in rarefied gases at lower computational cost.

There are two well-known approaches towards this goal, the Chapman–Enskog method^{1,2,6} and the method of moments of Grad.^{7–9}

In the Chapman–Enskog method, the phase density is expanded in powers of the Knudsen number Kn , defined as the ratio between the mean free path of the molecules and the relevant macroscopic length scale. To zeroth-order the expansion yields the Euler equations, the first-order correction results in the equations of Navier–Stokes and Fourier, the second-order expansion yields the Burnett equations,^{2,6} and the third-order expansion yields the so-called Super-Burnett equations.^{10,11} The equations of Navier–Stokes and Fourier cease to be accurate for Knudsen numbers above 0.05, and one is led to think that Burnett and Super-Burnett equations are valid for larger Knudsen numbers. Unfortunately, however, the higher order equations become linearly unstable for processes involving small wavelengths, or high frequencies, and thus cannot be used in numerical simulations.^{10,12} In recent years, several authors presented augmented forms of the Burnett equations that contain additional terms of Super-

Burnett order (but not the actual Super-Burnett terms) to stabilize the equations,^{13,14} or derived regularizations of hyperbolic equations that reproduce the Burnett equations when expanded in Kn .^{15–17}

In the method of moments of Grad,^{7,8} the Boltzmann equation is replaced by a set of moment equations—first-order partial differential equations for the moments of the distribution function. Which and how many moments are needed depends on the particular process, but experience shows that the number of moments must be increased with increasing Knudsen number.^{9,18–21} For the closure of the equations, the phase density is approximated by an expansion in Hermite polynomials about the equilibrium distribution (the local Maxwellian), where the coefficients are related to the moments.

Only few moments have an intuitive physical meaning, i.e., density ϱ , momentum density ϱv_i , energy density ϱe , heat flux q_i , and pressure tensor p_{ij} . This set of 13 moments²² forms the basis of Grad's well-known 13 moment equations⁷ which are commonly discussed in textbooks.²³ However, the 13 moment set does not allow the computation of boundary layers^{18,24,25} and, since the equations are symmetric hyperbolic, leads to shock structures with discontinuities (sub-shocks) for Mach numbers above 1.65.^{9,26} With increasing number of moments, one can compute Knudsen boundary layers^{18,27} and smooth shock structures up to higher Mach numbers.^{20,26} As becomes evident from the cited literature, for some problems, in particular for large Mach or Knudsen numbers, one has to face hundreds of moment equations.

In most of the available literature, both methods—moment method and Chapman–Enskog expansion—are treated as being completely unrelated. However, using a method akin to the Maxwellian iteration of Truesdell and Ikenberry,^{28,29} Reinecke and Kremer could extract the Bur-

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nett equation from Grad's 13 moment system.^{30–32} In Ref. 25 it was shown that their iteration method is equivalent to the Chapman–Enskog expansion of the moment equations. In the course of the present paper it will become clear that the Super-Burnett equations cannot be extracted from a set of 13 moment equations, but from a set with 26 moments.

In this paper we shall derive and discuss a set of equations for the 13 moments ϱ , ϱv_i , ϱe , q_i , $p_{(ij)}$ which is based on Grad's theory for 13 moments, and the corresponding distribution function, but differs from the established method in the closure relations. Our method adds some terms of Super-Burnett order to the usual 13 equations. The additional terms, which are obtained from the moment equations for higher moments, place the new equations in between the Super-Burnett and Grad's 13 moment equations in as much as the new equations keep the desirable features of both, while discarding the unwelcome features. In particular, the new equations:

- (i) Contain the Burnett and Super-Burnett equations as can be seen by means of a Chapman–Enskog expansion in the Knudsen number;
- (ii) are linearly stable for all wavelengths, and/or frequencies;
- (iii) show phase speeds and damping coefficients that match experiments better than those for the Navier–Stokes–Fourier equations, or the original 13 moments system;
- (iv) exhibit Knudsen boundary layers;
- (v) lead to smooth shock structures for all Mach numbers.

In the present paper we shall derive the new equations, and discuss the first three points above for the linearized equations in detail. Also, we shall show the existence of boundary layers, but shall not discuss how to obtain proper jump and slip boundary conditions for the equations. This problem, and the computation and discussion of the shock structure will be discussed in future papers.

Hyperbolic partial differential equations imply finite wave speeds and discontinuities that make them difficult to handle with standard analysis. Regularization is a method to add some parabolic terms which change the character of the equations so that no discontinuities occur, but a narrow smooth transition zone.^{33,34} We decided to adopt the notion of regularization for the new equations since the additional terms indeed are smoothing out the discontinuities (subshocks) that occur in Grad's 13 moment system for Mach numbers above 1.65. It is important to note, though, that the shocks in Grad's moment equations (at $Ma=1.65$ for 13 moments, at higher Mach numbers for extended moment sets, see Refs. 9 and 26) are artefacts of the method, and thus unphysical. The parameter that controls our regularization is the mean time of free flight, which is a physical parameter. In other words, the regularization of Grad's 13 moment system removes artificial discontinuities, and replaces them by a shock structure which is based in physics.

Simply put, the regularized equations follow from a Chapman–Enskog like procedure, where the expansion is performed about a nonequilibrium state, which is described

by the 13 moments. This idea was also presented by Karlin *et al.*³⁵ for the linearized Boltzmann equation. The main difference between our approach and the one of Karlin *et al.* lies in the fact that we base the derivation of the equations on the nonlinear moment equations, instead of the linearized Boltzmann equation, so that we obtain a set of nonlinear equations. Also, the use of moment equations allows for a much faster derivation of the equations, and yields explicit numerical expressions for coefficients that were not specified in Ref. 35. Thus, the Karlin *et al.* equations follow from our equations by linearization. Karlin *et al.* do not discuss the relation between their equations and the Burnett and Super-Burnett equations.

A thorough discussion of the orders of magnitude of moments (in the Chapman–Enskog sense) lead Müller *et al.*³⁶ to a new view on moment equations. In particular, they considered higher order iterations in the set of all moment equations in order to find the proper variables corresponding to a given order $\mathcal{O}(Kn^n)$. In their work they suggest a “possible parabolization” that is different in spirit, but very similar in fact to our method of regularization. Since the aim of that work lies in the discussion of orders of magnitude, the authors only considered special cases, i.e., one-dimensional flows,¹ or even a one-dimensional gas, and Bhatnagar–Gross–Krook (BGK) production terms, that allowed them to explicitly expand up to high orders. Due to these simplifications, it is not possible to compare their results with ours.

Jin and Slemrod presented a set of regularized Burnett equations^{16,17} which bear some resemblance to our set of equations. Their equations are constructed to guarantee the positivity of the entropy production, and contain several unknown parameters. At present, the relation between these equations and our new regularized equations is not clear. The advantage of our method is that it shows a rational path how to obtain regularizations for Grad moment systems with any number of moments. Additionally we recall that our equations contain no free parameters.

The remainder of the paper is organized as follows. In the next section we discuss moment equations in general, and derive the new set of equations. Section III deals with Chapman–Enskog expansions. We show that the expansion of the new equations yields the Burnett and Super-Burnett equations (in the linear case), and discuss the relation between Chapman–Enskog expansions, Grad's moment equations, and the new equations. In Sec. IV we consider plane wave solutions to prove the stability of the equations, and show that phase velocity and damping are in good agreement with experimental data for a large range of frequencies. The Knudsen boundary layers as predicted from the regularized moment equations are discussed in Sec. V. The paper ends with our conclusions.

II. MOMENT SYSTEMS

A. Grad's moment method

We consider monatomic ideal gases. The objective of the kinetic theory of gases is the determination of the phase density $f(x_i, t, c_i)$ which gives the number of particles in the phase space element $dx dc$. Here, x_i, t denote space and time

variables, respectively, and c_i is the velocity of a particle of mass m . The phase density is governed by the Boltzmann equation^{1,2}

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = \mathcal{S}(f), \quad (1)$$

where the collision term $\mathcal{S}(f)$ accounts for the change of the phase density due to collisions among particles. \mathcal{S} depends on the interaction potential between particles, and in the present paper we shall mainly consider Maxwell molecules,² and a slight modification thereof, see Sec. IID below.

Once the phase density is known, one may calculate its moments, for instance the mass density ϱ , the momentum density ϱv_i and the thermal energy density $\varrho \varepsilon$, given by

$$\begin{aligned} \varrho &= m \int f \, d\mathbf{c}, \quad \varrho v_i = m \int c_i f \, d\mathbf{c}, \\ \varrho \varepsilon &= \frac{3}{2} \varrho \frac{k}{m} T = \frac{m}{2} \int C^2 f \, d\mathbf{c}. \end{aligned} \quad (2)$$

In these definitions, k is Boltzmann's constant, v_i denotes the barycentric velocity of the gas, $C_i = c_i - v_i$ is the peculiar velocity, and T denotes the temperature, which is defined here.

Pressure tensor p_{ij} and heat flux vector q_i are given by

$$\begin{aligned} p_{ij} &= p \delta_{ij} + p_{\langle ij \rangle} = p \delta_{ij} + \sigma_{ij} = m \int C_i C_j f \, d\mathbf{c}, \\ q_i &= \frac{m}{2} \int C^2 C_i f \, d\mathbf{c}. \end{aligned}$$

By comparison with (2) the pressure is related to temperature and density by the ideal gas law, $p = \varrho (k/m) T$. The pressure deviator is denoted by $p_{\langle ij \rangle} = \sigma_{ij}$; here, and in the following, the angular brackets label the traceless part of a symmetric tensor.

In moment methods one assumes that the state of the gas is satisfactorily described by a set of N moments

$$\rho_A = \int \Psi_A(C_k) f \, d\mathbf{c}, \quad A = 1, \dots, N, \quad (3)$$

where $\Psi_A(C_k)$ is a vector of polynomials of the peculiar velocity. In Grad's 13 moment theory one has $\Psi_A = m\{1, c_i, \frac{1}{2}C^2, C_{\langle i} C_{j \rangle}, \frac{1}{2}C^2 C_{ij}\}$, i.e., the moments $\varrho, \varrho v_i, \varrho \varepsilon, p_{\langle ij \rangle}, q_i$ defined above are the variables under consideration.

Multiplication of the Boltzmann equation (1) by Ψ_A and subsequent integration over velocity space yields the moment equations

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial(\rho_A v_k + \rho_{Ak})}{\partial x_k} - \int \left(\frac{\partial \Psi_A}{\partial t} + c_k \frac{\partial \Psi_A}{\partial x_k} \right) f \, d\mathbf{c} = P_A, \quad (4)$$

with

$$\rho_{Ak} = \int \Psi_A C_k f \, d\mathbf{c}, \quad P_A = \int \Psi_A \mathcal{S} f \, d\mathbf{c}.$$

Equations (4)₁ do not form a closed system of partial differential equations for the moments since they contain some

higher order moments ρ_{Ak} that are not among the variables (3), as well as the productions P_A . The integrals of the derivatives of Ψ_A can be expressed in terms of the variables ρ_A . In order to close the system for the variables ρ_A , a closure assumption is required that allows to relate the additional moments and the productions to the variables.

In Grad's moment method, the phase density is related to the moments as

$$f|_N = f_M \left(1 + \sum_{A=1}^N \Lambda_A(\rho_B) \Psi_A \right) \quad (5)$$

with

$$\rho_A = \int \Psi_A f|_N \, d\mathbf{c}, \quad A = 1, \dots, N,$$

where the coefficients Λ_A follow from the inversion of the last equation.^{7,8} f_M denotes the local Maxwellian, given by

$$f_M = \frac{\varrho}{m} \sqrt{\frac{m}{2\pi kT}}^3 e^{-(m/2kT) C^2}.$$

Equation (5) will be used to compute the constitutive functions for higher moments and productions as

$$\rho_{Ak}(x_i, t) = \rho_{Ak}(\rho_B(x_i, t)), \quad P_A(x_i, t) = P_A(\rho_B(x_i, t)).$$

The constitutive functions are local, i.e., depend only on the local values of the moments ρ_A , and not on gradients or time derivatives of the moments.

B. 13 moment equations and their regularization

Now we specify the above formalism for the 13 moment system. The basic equations for the 13 moments $\rho_A = \{\varrho, \varrho v_i, \varrho \varepsilon = \frac{3}{2} \varrho (k/m) T, \sigma_{ij}, q_i\}$ read

$$\begin{aligned} \frac{\partial \varrho}{\partial t} + \frac{\partial \varrho v_k}{\partial x_k} &= 0, \\ \varrho \frac{\partial v_i}{\partial t} + \varrho v_k \frac{\partial v_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} &= 0, \end{aligned} \quad (6)$$

$$\begin{aligned} \frac{3}{2} \varrho \frac{\partial T}{\partial t} + \frac{3}{2} \varrho v_k \frac{\partial T}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + p \frac{\partial v_k}{\partial x_k} + \sigma_{ij} \frac{\partial v_i}{\partial x_j} &= 0, \\ \frac{\partial \sigma_{ij}}{\partial t} + \frac{\partial \sigma_{ij} v_k}{\partial x_k} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} + \frac{\partial \rho_{\langle ijk \rangle}}{\partial x_k} + 2p \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} + 2\sigma_{k\langle i} \frac{\partial v_{j \rangle}}{\partial x_k} &= -\frac{\sigma_{ij}}{\tau}, \end{aligned} \quad (7)$$

$$\begin{aligned} \frac{\partial q_i}{\partial t} + \frac{\partial q_i v_k}{\partial x_k} + \frac{1}{2} \frac{\partial \rho_{rr\langle ik \rangle}}{\partial x_k} + \frac{1}{6} \frac{\partial \rho_{rrss}}{\partial x_i} - \frac{5}{2} \frac{p}{\varrho} \frac{\partial p}{\partial x_i} - \frac{5}{2} \frac{p}{\varrho} \frac{\partial \sigma_{ik}}{\partial x_k} &= -\frac{\sigma_{ik}}{\varrho} \frac{\partial p}{\partial x_k} - \frac{\sigma_{ij}}{\varrho} \frac{\partial \sigma_{jk}}{\partial x_k} + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2}{5} q_k \frac{\partial v_k}{\partial x_i} + \frac{2}{5} q_i \frac{\partial v_k}{\partial x_k} \\ + \rho_{\langle ijk \rangle} \frac{\partial v_j}{\partial x_k} &= -\frac{2}{3} \frac{q_i}{\tau}. \end{aligned} \quad (8)$$

The first five equations, i.e., the set (6)_{1,2,3}, are the conservation laws for mass, momentum and energy, while Eqs. (7)

and (8) are the respective balance laws for the pressure deviator and the heat flux vector. For the computation of the production terms on the right-hand sides, we have assumed Maxwell molecules. In particular, τ is the collision time, which for Maxwell molecules is given by $\tau=1/(\varrho\alpha)$ where α is a constant. We shall discuss the relation between τ and viscosity below, in Sec. IID, where we shall present a modification that allows the extension of the model to other types of interaction.

Equations (6), (7), and (8) do not form a closed set of equations, since they contain the additional quantities $\rho_{\langle ijk \rangle}$, $\rho_{rr\langle ij \rangle}$, and ρ_{rrss} , which must be related to the variables via the distribution function. For the variables at hand, the Grad distribution (5) reads

$$f_{|13} = f_M \left(1 + \frac{m^2}{2\varrho k^2 T^2} \sigma_{jk} C_{\langle j} C_k \right) - \frac{m^2}{\varrho k^2 T^2} q_k C_k \left(1 - \frac{1}{5} \frac{m}{kT} C^2 \right), \tag{9}$$

and from this function one computes

$$\rho_{\langle ijk \rangle|13} = 0, \quad \rho_{rr\langle ij \rangle|13} = 7 \frac{k}{m} T \sigma_{ij}, \quad \rho_{rrss|13} = 15 \frac{p^2}{\varrho}. \tag{10}$$

Insertion of these relations into (7) and (8) yields Grad's well-known system for 13 moments.⁷ This system is symmetric hyperbolic for a wide range of values of the variables,⁹ and develops discontinuous shocks for Mach numbers above 1.65.

In order to regularize this system, we define the deviations of $\rho_{\langle ijk \rangle}$, $\rho_{rr\langle ij \rangle}$, and ρ_{rrss} from their values obtained with the Grad closure (10) as

$$m_{ijk} = \rho_{\langle ijk \rangle} - \rho_{\langle ijk \rangle|13} = \rho_{\langle ijk \rangle},$$

$$R_{ij} = \rho_{rr\langle ij \rangle} - \rho_{rr\langle ij \rangle|13} = \rho_{rr\langle ij \rangle} - 7 \frac{k}{m} T \sigma_{ij}, \tag{11}$$

$$\Delta = \rho_{rrss} - \rho_{rrss|13} = \rho_{rrss} - 15 \frac{p^2}{\varrho}.$$

For the Grad closure we thus have $m_{ijk} = R_{ik} = \Delta = 0$. We proceed by computing nonzero approximations for these quantities that follow from the moment equations for $\rho_{\langle ijk \rangle}$, $\rho_{rr\langle ik \rangle}$, and ρ_{rrss} , which are given in Appendix A. In these equations, the quantities m_{ijk} , R_{ik} , and Δ are introduced according to Eqs. (11) and all time derivatives of the 13 variables $\{\varrho, \varrho v_i, \varrho \varepsilon = \frac{3}{2} \varrho (k/m) T, \sigma_{ij}, q_i\}$ are eliminated by means of their corresponding balance laws (6), (7), and (8). After some algebra, one obtains equations that can be written in short as

$$\frac{\partial m_{ijk}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{3}{2} \frac{m_{ijk}}{\tau},$$

$$\frac{\partial R_{ij}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{7}{6} \frac{R_{ij}}{\tau},$$

$$\frac{\partial \Delta}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{2}{3} \frac{\Delta}{\tau}, \tag{12}$$

where—again—the production terms on the right are computed for Maxwell molecules.

For the sake of the argument, we assume that the non-equilibrium moments of the 13 field case, i.e., σ_{ij} and q_i , change on the time scale defined by τ , while all other non-equilibrium moments change on a faster time scale $\varepsilon\tau$ where ε is “small.” Indeed, we consider ε as a formal smallness parameter that will be set equal to one at the end of the calculations. In this case, Eqs. (12) are slightly changed on the right hand side which now contains the parameter ε

$$\frac{\partial m_{ijk}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{1}{\varepsilon} \frac{3}{2} \frac{m_{ijk}}{\tau},$$

$$\frac{\partial R_{ij}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{1}{\varepsilon} \frac{7}{6} \frac{R_{ij}}{\tau},$$

$$\frac{\partial \Delta}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{1}{\varepsilon} \frac{2}{3} \frac{\Delta}{\tau}. \tag{13}$$

Similar equations can be written for all higher moments. These equations are now expanded in terms of the parameter ε as

$$m_{ijk} = m_{ijk}^{(0)} + \varepsilon m_{ijk}^{(1)} + \dots, \quad R_{ij} = R_{ij}^{(0)} + \varepsilon R_{ij}^{(1)} + \dots, \tag{14}$$

$$\Delta = \Delta^{(0)} + \varepsilon \Delta^{(1)} + \dots,$$

where we only account for terms up to order $\mathcal{O}(\varepsilon)$. This procedure is a Chapman–Enskog like expansion with ε as smallness parameter.

The constitutive laws for m_{ijk} , R_{ik} , and Δ result from inserting the ansatz (14) into Eqs. (13), and balancing terms of the same order in ε . It is straightforward to see that the zeroth-order approximation (balancing terms with the factor $1/\varepsilon$) just gives Grad's 13 moment case, corresponding to

$$m_{ijk}^{(0)} = R_{ij}^{(0)} = \Delta^{(0)} = 0.$$

The first-order corrections result from balancing terms of order ε^0 and can be written as

$$\left[\frac{\partial m_{ijk}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} \right]_{|f_{13}} = -\frac{3}{2} \frac{m_{ijk}^{(1)}}{\tau},$$

$$\left[\frac{\partial R_{ij}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} \right]_{|f_{13}} = -\frac{7}{6} \frac{R_{ij}^{(1)}}{\tau},$$

$$\left[\frac{\partial \Delta}{\partial t} + \{ \dots \text{space derivatives of moments} \dots \} \right]_{|f_{13}}$$

$$= -\frac{2}{3} \frac{\Delta^{(1)}}{\tau},$$

where the notation $[\cdot]_{|f_{13}}$ indicates that *all* moments in *all* terms inside the square brackets must be evaluated with the phase density $f_{|13}$ as given in Eq. (9), that is by

$$\rho_{\langle ijkl \rangle |13} = \rho_{\langle ijkl \rangle |13} = \rho_{rr\langle ijkl \rangle |13} = 0, \quad \rho_{rr\langle ij \rangle |13} = 7 \frac{k}{m} T \sigma_{ij},$$

$$\rho_{rrrs |13} = 15 \frac{p^2}{\rho}, \quad \text{and} \quad m_{ijk |13} = R_{ij |13} = \Delta_{|13} = 0.$$

The result can be summarized as follows.

The corrections to Grad’s 13 moment equations read (after setting $\varepsilon = 1$)

$$m_{ijk} = m_{ijk}^{(1)} = -2\tau \left[\frac{k}{m} T \frac{\partial \sigma_{\langle ij \rangle}}{\partial x_k} - \frac{k}{m} T \sigma_{\langle ij \rangle} \frac{\partial \ln \varrho}{\partial x_k} + \frac{4}{5} q_{\langle i} \frac{\partial v_j}{\partial x_k} - \frac{\sigma_{\langle ij \rangle}}{\varrho} \frac{\partial \sigma_{k \rangle l}}{\partial x_l} \right],$$

$$R_{ij} = R_{ij}^{(1)} = -\frac{24}{5} \tau \left[\frac{k}{m} T \frac{\partial q_{\langle i}}{\partial x_j} + \frac{k}{m} q_{\langle i} \frac{\partial T}{\partial x_j} - \frac{k}{m} T q_{\langle i} \frac{\partial \ln \varrho}{\partial x_j} - \frac{1}{\rho} q_{\langle i} \frac{\partial \sigma_{j \rangle k}}{\partial x_k} + \frac{5}{7} \frac{k}{m} T \left(\sigma_{k \langle i} \frac{\partial v_j \rangle}{\partial x_k} + \sigma_{k \langle i} \frac{\partial v_k}{\partial x_j} - \frac{2}{3} \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right) - \frac{5}{6} \frac{\sigma_{ij}}{\varrho} \frac{\partial q_k}{\partial x_k} - \frac{5}{6} \frac{\sigma_{ij}}{\varrho} \sigma_{kl} \frac{\partial v_k}{\partial x_l} \right], \tag{15}$$

$$\Delta = \Delta^{(1)} = -12\tau \left[\frac{k}{m} T \frac{\partial q_k}{\partial x_k} + \frac{5}{2} \frac{k}{m} q_k \frac{\partial T}{\partial x_k} - \frac{k}{m} T q_k \frac{\partial \ln \varrho}{\partial x_k} - \frac{1}{\varrho} q_j \frac{\partial \sigma_{jk}}{\partial x_k} + \frac{k}{m} T \sigma_{ij} \frac{\partial v_i}{\partial x_j} \right].$$

These must be inserted into the equations for pressure deviator and heat flux vector which read

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{\partial \sigma_{ij} v_k}{\partial x_k} + \frac{4}{5} \frac{\partial q_{\langle i}}{\partial x_j} + 2p \frac{\partial v_{\langle i}}{\partial x_j} + 2\sigma_{k \langle i} \frac{\partial v_j \rangle}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k} = -\frac{\sigma_{ij}}{\tau}, \tag{16}$$

$$\frac{\partial q_i}{\partial t} + \frac{\partial q_i v_k}{\partial x_k} + \frac{5}{2} p \frac{\partial \frac{k}{m} T}{\partial x_i} + \frac{5}{2} \sigma_{ik} \frac{\partial \frac{k}{m} T}{\partial x_k} + \frac{k}{m} T \frac{\partial \sigma_{ik}}{\partial x_k} - \sigma_{ik} \frac{k}{m} T \frac{\partial \ln \varrho}{\partial x_k} - \frac{\sigma_{ij}}{\varrho} \frac{\partial \sigma_{jk}}{\partial x_k} + \frac{7}{5} q^k \frac{\partial v_i}{\partial x_k} + \frac{2}{5} q^k \frac{\partial v_k}{\partial x_i} + \frac{2}{5} q_i \frac{\partial v_k}{\partial x_k} + \frac{1}{2} \frac{\partial R_{ik}}{\partial x_k} + \frac{1}{6} \frac{\partial \Delta}{\partial x_i} + m_{ijk} \frac{\partial v_j}{\partial x_k} = -\frac{2}{3} \frac{q_i}{\tau}. \tag{17}$$

With these equations, we have derived the complete set of regularized equations for the 13 variables $\varrho, T, v_i, \sigma_{ij}, q_i$ that consists of Eqs. (6), (16), (17), and (15). In the next section, we shall discuss some of the background of the derivation.

In the following, we shall refer to these equations as the R13 equations, where “R” stands for “regularized,” and 13 denotes the number of variables. In Sec. IID, we shall show that the Navier–Stokes–Fourier equations might be denoted as the R5 equations.

C. A closer look on the derivation of Grad’s equations and the R13 equations

It is well known that the relaxation times for moments grow only slowly,³⁹ so that the relaxation times of the first 26 moments are of the same magnitude τ . This becomes obvious by a glance at the right hand sides of Eqs. (12) where the factors $\{3/2 1/\tau, 7/6 1/\tau, 2/3 1/\tau\}$ define the respective time scales for the moments. Accordingly, the parameter ε is not small, but of order unity. Thus, the basic assumption in our derivation—the smallness of ε —is not well justified. Nevertheless, the argument shows that the assumption behind the R13 equations, which require ε as “small,” is less restrictive than the the assumption behind Grad’s 13 moment system which requires $\varepsilon = 0$.

The great advantage of our method is that it is based on a Chapman–Enskog expansion of only *first order* to obtain a set of equations which agrees with the Boltzmann equation to a *higher order*, as we shall show in Sec. III. It is well-known that the first order Chapman–Enskog expansion yields stable equations, while expansions to higher order yield unstable equations, see Refs. 10 and 40 and Sec. IV B.

Nevertheless, a full Chapman–Enskog expansion in Kn of the infinite moment system reveals more information about the order of magnitude of the moments. In Ref. 36 a high order expansion (again, termed as Maxwell iteration) showed indeed that higher moments (that is moments of higher powers in velocity) are of higher order in the Knudsen number in the Chapman–Enskog sense. For one-dimensional geometries, and for BGK production terms, the authors of that study were able to state which set of moments is appropriate for a given order of accuracy $\mathcal{O}(\text{Kn}^n)$.

Thus, a high order of accuracy requires more moments. Since equations obtained from the Chapman–Enskog expansion are unstable if orders higher than one are accounted for, the expansion can only give hints which moments to use, but not which equations. Grad’s sets of moment equations are a better choice, since they are linearly stable, and well-posed. However, their hyperbolicity implies finite speeds leading to unphysical sub-shocks for larger Mach numbers, and one must conclude that they are restricted in validity as well. The R13 equations seem to be the best choice, as they combine the desirable features of both approaches.

In the same paper, Ref. 36, a possible regularization of moment equations is presented. While the spirit of that work seems quite different from the present approach, the idea of regularization is very similar. The results are not easy to compare, since in Ref. 36 the authors do not consider moments, but Hermite polynomials, have BGK production

terms instead of those for Maxwell molecules, and do not relate their systems of equations to sets of moment equations, nor higher order Chapman–Enskog expansions.

D. Euler and Navier–Stokes equations

In this section, we use the same method of regularization in order to derive the equations of Navier–Stokes and Fourier which can be considered as the regularization of the Euler equations. This section is intended to show the reader that the very same idea that resulted in the R13 equations can be used to derive a familiar result. Besides, the Navier–Stokes equations allow us to relate the microscopic parameter $\alpha = 1/(\varrho \tau)$ to viscosity data.

Indeed, the first member of the meaningful sets of Grad type moment equations is the 5 moments case, better known as Euler equations, where $\Psi_A = m\{1, c_i, \frac{1}{2}C^2\}$, corresponding to the five variables $\rho_A = \{\varrho, \varrho v_i, \varrho \varepsilon = \frac{3}{2}\varrho (k/m) T\}$ or $\{\varrho, v_i, T\}$. Accordingly, the relevant moment equations are the conservation laws for mass, momentum and energy (6). Of course, these five equations are not a closed set for the five variables $\{\varrho, v_i, T\}$ since they contain the pressure deviator σ_{ij} and the heat flux vector q_i . Straightforward application of the Grad closure (5) reveals that the corresponding distribution function for the closure is the Maxwellian, $f|_5 = f_M$, which yields

$$\sigma_{ij|5} = 0 \quad \text{and} \quad q_{i|5} = 0. \tag{18}$$

The resulting equations are the well-known Euler equations for an ideal gas. In particular, the Euler equations are of hyperbolic nature and exhibit discontinuous shocks in supersonic flow problems.

For the regularization we introduce the smallness parameter ε in the right-hand sides of the balances for σ_{ij} and q_i , Eqs. (7) and (18), which then read

$$\frac{\partial \sigma_{ij}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{1}{\varepsilon} \frac{\sigma_{ij}}{\tau},$$

$$\frac{\partial q_i}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} = -\frac{1}{\varepsilon} \frac{2}{3} \frac{q_i}{\tau}.$$

Next, we make the ansatz

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \varepsilon \sigma_{ij}^{(1)}, \quad q_i = q_i^{(0)} + \varepsilon q_i^{(1)},$$

and equate terms of equal powers in ε . As can be expected, we find

$$\sigma_{ij}^{(0)} = q_i^{(0)} = 0,$$

so that the zeroth-order expansion results in the Euler equations. The first-order expansion yields

$$\left[\frac{\partial \sigma_{ij}}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} \right]_{|f_5} = -\frac{1}{\varepsilon} \frac{\sigma_{ij}^{(1)}}{\tau},$$

$$\left[\frac{\partial q_i}{\partial t} + \{\dots \text{space derivatives of moments} \dots\} \right]_{|f_5} = -\frac{1}{\varepsilon} \frac{2}{3} \frac{q_i^{(1)}}{\tau},$$

where all moments in the square brackets must be replaced by their values computed with the Maxwellian $f|_5 = f_M$, that is from the Grad function for the case under consideration. These values are easily computed as

$$\sigma_{ij|5} = q_{i|5} = \rho_{(ijk)|5} = \rho_{rr(ij)|5} = 0 \quad \text{and} \quad \rho_{rrss|5} = 15 \frac{p^2}{\varrho},$$

and it follows that the two equations simply reduce to the Navier–Stokes law for the stress tensor, and the Fourier law for the heat flux

$$\sigma_{ij} = \sigma_{ij}^{(1)} = -2\mu \frac{\partial v_{(i}}{\partial x_{j)}}, \quad q_i = q_i^{(1)} = -\kappa \frac{\partial T}{\partial x_i}. \tag{19}$$

Here, μ and κ denote viscosity and heat conductivity, respectively, and are given as

$$\mu = \tau p = \frac{p}{\varrho \alpha} = \frac{k}{m} \frac{T}{\alpha}, \quad \kappa = \frac{15}{4} \tau p \frac{k}{m} = \frac{15}{4} \frac{k}{m} \mu.$$

While the viscosity is linear in T for Maxwell molecules, one finds for more realistic interaction potentials a relation of the form

$$\mu = \mu_0 \left(\frac{T}{T_0} \right)^s,$$

where μ_0 is a reference value measured at T_0 and s is a constant in the interval $[0.5, 1]$. In particular, one finds $s = 1$ for Maxwell molecules, and $s = 0.5$ for hard spheres. See Ref. 4 for more details and tables for the appropriate values of μ_0 and s for various gases. While we use the production terms for Maxwell molecules throughout this paper, we generalize the approach by setting

$$\alpha = \frac{k}{m} \frac{T}{\mu_0} \left(\frac{T_0}{T} \right)^s,$$

in order to have a more accurate description of the gas. For Maxwell molecules one has $s = 1$, hence $\alpha = \text{const}$, while for argon $s \approx 0.8$ gives good agreement with experimental data.

As is well known, the Navier–Stokes–Fourier (NSF) equations are not hyperbolic, and do not allow discontinuous shocks. Thus, the NSF equations can be considered as the regularization of the Euler equations.

E. Linearized equations

In the remainder of this paper, we shall discuss the R13 equations only for small deviations from an equilibrium state given by $\varrho_0, T_0, v_{i,0} = 0$. Dimensionless variables $\hat{\varrho}, \hat{T}, \hat{v}_i, \hat{\sigma}_{ij}, \hat{q}$ are introduced as

$$\varrho = \varrho_0(1 + \hat{\varrho}), \quad T = T_0(1 + \hat{T}),$$

$$p = \varrho_0 \frac{k}{m} T_0(1 + \hat{\varrho} + \hat{T}), \quad v_i = \sqrt{\frac{k}{m} T_0} \hat{v}_i,$$

$$\sigma_{ij} = \varrho_0 \frac{k}{m} T_0 \hat{\sigma}_{ij}, \quad q_i = \varrho_0 \left(\sqrt{\frac{k}{m} T_0} \right)^3 \hat{q}_i.$$

Moreover, we identify a relevant length scale L of the process, and use it to nondimensionalize the space and time variables according to

$$x_i = L \hat{x}_i, \quad t = \frac{L}{\sqrt{\frac{k}{m} T_0}} \hat{t}.$$

The corresponding dimensionless collision time is then given by the Knudsen number, which we define here as

$$\text{Kn} = \frac{\tau \sqrt{\frac{k}{m} T_0}}{L} = \frac{\mu_0 \sqrt{\frac{k}{m} T_0}}{\rho_0 L}. \tag{20}$$

It must be mentioned that the definition of the Knudsen number varies in the literature; definitions frequently used are $\text{Kn}' = \sqrt{(\pi/2)} \text{Kn}^1$ and $\text{Kn}'' = \frac{8}{5} \sqrt{(2/\pi)} \text{Kn}$,⁴ our definition (20) was chosen for notational convenience.

Linearization in the deviations from equilibrium $\hat{\varrho}$, \hat{T} , \hat{v}_i , $\hat{\sigma}_{ij}$, \hat{q} yields the dimensionless linearized system in three dimensions as

$$\frac{\partial \hat{\varrho}}{\partial \hat{t}} + \frac{\partial \hat{v}_k}{\partial \hat{x}_k} = 0,$$

$$\frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\varrho}}{\partial \hat{x}_i} + \frac{\partial \hat{T}}{\partial \hat{x}_i} + \frac{\partial \hat{\sigma}_{ik}}{\partial \hat{x}_k} = 0,$$

$$\frac{3}{2} \frac{\partial \hat{T}}{\partial \hat{t}} + \frac{\partial \hat{q}_k}{\partial \hat{x}_k} + \frac{\partial \hat{v}_k}{\partial \hat{x}_k} = 0,$$

$$\begin{aligned} \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{t}} + \frac{4}{5} \frac{\partial \hat{q}_{\langle i}}{\partial \hat{x}_{j \rangle}} + 2 \frac{\partial \hat{v}_{\langle i}}{\partial \hat{x}_{j \rangle}} - 2 \text{Kn} \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{\sigma}_{\langle ij \rangle}}{\partial \hat{x}_k} &= - \frac{\hat{\sigma}_{ij}}{\text{Kn}}, \\ \frac{\partial \hat{q}_i}{\partial \hat{t}} + \frac{5}{2} \frac{\partial \hat{T}}{\partial \hat{x}_i} + \frac{\partial \hat{\sigma}_{ik}}{\partial \hat{x}_k} - \frac{12}{5} \text{Kn} \frac{\partial}{\partial \hat{x}_k} \frac{\partial \hat{q}_{\langle i}}{\partial \hat{x}_{k \rangle}} - 2 \text{Kn} \frac{\partial}{\partial \hat{x}_i} \frac{\partial \hat{q}_k}{\partial \hat{x}_k} \\ &= - \frac{2}{3} \frac{\hat{q}_i}{\text{Kn}}. \end{aligned} \tag{21}$$

This set of equations is equivalent to the equations proposed by Karlin *et al.*,³⁵ who—however—did not give explicit numerical expressions for the factors that multiply the second derivatives of $\hat{\sigma}_{ij}$ and \hat{q}_i , but presented them as integrals over the linearized collision operator which are not further evaluated.

The hats will be omitted in the sequel.

III. CHAPMAN–ENSKOG EXPANSIONS

A. Burnett and Super-Burnett limits

We proceed by showing that the Chapman–Enskog expansion of the linearized system (21) gives the linear Burnett and Super-Burnett equations. In Refs. 25 and 31 it was shown that the expansion of the full nonlinear 13 moment equations yields the nonlinear Burnett equations. The additional quantities m_{ijk} , R_{ik} , and Δ correspond to third-order corrections to σ_{ij} and q_i , and therefore are of Super-Burnett order. Accordingly, the full R13 equations contain the nonlinear Burnett equations as well. The complete Super-Burnett equations are almost never used, and hard to find in the literature.^{10,11} Their derivation is quite cumbersome, and that is the reason why we restrict ourselves to the linear case.

The idea of the Chapman–Enskog expansion is to expand the distribution function in a series in the Knudsen number as

$$f = f^{(0)} + \text{Kn} f^{(1)} + \text{Kn}^2 f^{(2)} + \text{Kn}^3 f^{(3)} + \dots,$$

where the $f^{(\alpha)}$ are obtained from the Boltzmann equation.^{2,37} In our case, we operate on the level of moments and moment equations, and thus we expand pressure deviator and heat flux in a series as

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \text{Kn} \sigma_{ij}^{(1)} + \text{Kn}^2 \sigma_{ij}^{(2)} + \text{Kn}^3 \sigma_{ij}^{(3)} + \dots,$$

$$q_i = q_i^{(0)} + \text{Kn} q_i^{(1)} + \text{Kn}^2 q_i^{(2)} + \text{Kn}^3 q_i^{(3)} + \dots.$$

Note that in the Chapman–Enskog expansion, opposed to the Hilbert expansion, the equilibrium variables ϱ, v_i, T are not expanded.^{2,37} The above expressions are inserted into the balance equations (21)_{4,5} and terms with equal powers in Kn are equated to find the $\sigma_{ij}^{(\alpha)}$, $q_i^{(\alpha)}$.

Here, it is customary, to express the time derivatives of $\sigma_{ij}^{(\alpha)}$, $q_i^{(\alpha)}$ by time derivatives of the hydrodynamic variables ϱ, T, v_i , this must be done successively as described below.

Considering the terms of order $\mathcal{O}(\text{Kn}^{-1})$, we find

$$\sigma_{ij}^{(0)} = q_i^{(0)} = 0. \tag{22}$$

This is the zeroth-order solution that corresponds to the Euler equations, see Eq. (18).

Equating the terms of order $\mathcal{O}(\text{Kn}^0)$, we find

$$\sigma_{ij}^{(1)} = -2 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \quad \text{and} \quad q_i^{(1)} = - \frac{15}{4} \frac{\partial T}{\partial x_i}, \tag{23}$$

i.e., the laws of Navier–Stokes and Fourier, Eq. (19), which therefore, form the first-order correction to the Euler equations.

Before the next step, the time derivatives of $\sigma_{ij}^{(1)}$, $q_i^{(1)}$ must be replaced by means of the balances of momentum and energy. With the result given in Appendix B, Eqs. (B1), we can then equate terms of order $\mathcal{O}(\text{Kn}^1)$ to obtain the linear Burnett (i.e., the second order) corrections as

$$\sigma_{ij}^{(2)} = -2 \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j \rangle}} + \frac{\partial^2 T}{\partial x_{\langle i} \partial x_{j \rangle}}$$

and

$$q_i^{(2)} = -\frac{13}{4} \frac{\partial^2 v_k}{\partial x_k \partial x_i} + \frac{3}{2} \frac{\partial^2 v_i}{\partial x_k \partial x_k}. \tag{24}$$

Again, the time derivatives of these expressions must be eliminated, see Eqs. (B2) in Appendix B, and then we find from the $\mathcal{O}(\text{Kn}^2)$ terms the linear Super-Burnett (i.e., the third order) contributions as

$$\sigma_{ij}^{(3)} = \frac{5}{3} \frac{\partial^2}{\partial x_{\langle i} \partial x_{j \rangle}} \frac{\partial v_k}{\partial x_k} - \frac{4}{3} \frac{\partial^2}{\partial x_k \partial x_k} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}}$$

and

$$q_i^{(3)} = -\frac{157}{16} \frac{\partial^3 T}{\partial x_i \partial x_k \partial x_k} - \frac{5}{8} \frac{\partial^3 \rho}{\partial x_i \partial x_k \partial x_k}. \tag{25}$$

These are the same equations that Shavaliyev found from the Boltzmann equation for Maxwell molecules.¹¹ The corresponding result for the one-dimensional case was also given by Bobylev.¹⁰

B. Discussion

From the previous paragraph follows that the R13 equations contain the Navier–Stokes–Fourier, Burnett, and Super-Burnett equations when expanded in the appropriate order in Kn.

The discussion of the preceding section also confirms that the newly added terms are of Super-Burnett order. Since these are based on the moment equations for $\rho_{\langle ij k \rangle}$, $\rho_{rr \langle ij \rangle}$ and ρ_{rrss} , we conclude that 26 moment equations are needed to produce the Super-Burnett equations.

We therefore see that the regularization improves the Chapman–Enskog order of accuracy: The regularization of the Euler equations which are $\mathcal{O}(\text{Kn}^0)$ adds terms of order $\mathcal{O}(\text{Kn})$ to yield the Navier–Stokes–Fourier equations. The regularization of the 13 moment equations which are accurate up to Burnett order $\mathcal{O}(\text{Kn}^2)$ adds third-order terms $\mathcal{O}(\text{Kn}^3)$.

The expansion procedure can be continued ad infinitum, with $\sigma_{ij}^{(\alpha)} \neq 0$, $q_i^{(\alpha)} \neq 0$ for all α . Of course, the $\sigma_{ij}^{(\alpha)}$, $q_i^{(\alpha)}$ for $\alpha \geq 4$ do not yield the correct expressions of the Chapman–Enskog expansion to order α , since terms from other (higher) moment equations will enter the proper expressions. Nevertheless, there are contributions of all orders $\mathcal{O}(\text{Kn}^\alpha)$, $\alpha = 1, \dots, \infty$, present in the R13 equations. It is in these higher order contributions that the R13 equations differ from the Burnett and Super-Burnett equations.

The regularization of the moment equations is a straightforward procedure that can be performed similarly on moment systems with more than 13 moments. A natural choice for the next system to consider would be to add the moments $\rho_{\langle ij k \rangle}$, $\rho_{rr \langle ij \rangle}$, and ρ_{rrss} to the list of variables, and then find the regularized closure conditions from even higher moment equations. This procedure would yield the R26 equations, and would need 45 moment equations to be derived. Presumably, the Chapman–Enskog expansion of the R26 equations will be accurate up to $\mathcal{O}(\text{Kn}^4)$, corresponding to the Super²-Burnett equations.

At this point it is worthwhile to mention that the computation of high-order Chapman–Enskog expansions of the

Boltzmann equation is forbiddingly complicated. The derivation of moment equations is much easier, and can be performed with help of computer algebra systems, see Ref. 38. Thus, it is imaginable, indeed, to compute and solve R26 or R45 moment equations, while it seems almost impossible to compute their Chapman–Enskog counterparts. Moreover, as the discussion in the next section will show, the R13 equations are superior to the higher-order Chapman–Enskog expansion, since they are stable.

IV. LINEAR ANALYSIS

A. Plane harmonic waves

In this section we consider the stability of the linearized R13 equations, for the case of one-dimensional processes where all variables depend only on $x_1 = x$, and where $v_i = \{v(x, t), 0, 0\}$. With $\sigma = \sigma_{11}$ and $q = q_1$, the equations reduce to

$$\begin{aligned} \frac{\partial \varrho}{\partial t} + \frac{\partial v}{\partial x} &= 0, \\ \frac{\partial v}{\partial t} + \frac{\partial \varrho}{\partial x} + \frac{\partial T}{\partial x} + \frac{\partial \sigma}{\partial x} &= 0, \\ \frac{3}{2} \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} + \frac{\partial v}{\partial x} &= 0, \\ \frac{\partial \sigma}{\partial t} + \frac{8}{15} \frac{\partial q}{\partial x} + \frac{4}{3} \frac{\partial v}{\partial x} - \frac{6}{5} \text{Kn} \frac{\partial^2 \sigma}{\partial x^2} &= -\frac{\sigma}{\text{Kn}}, \\ \frac{\partial q}{\partial t} + \frac{5}{2} \frac{\partial T}{\partial x} + \frac{\partial \sigma}{\partial x} - \frac{18}{5} \text{Kn} \frac{\partial^2 q}{\partial x^2} &= -\frac{2}{3} \frac{q}{\text{Kn}}. \end{aligned} \tag{26}$$

For comparison, we shall also consider the Chapman–Enskog expansion to various orders, in which case we have to replace the last two equations with the relevant terms of

$$\begin{aligned} \sigma_{CE} &= -\text{Kn} \frac{4}{3} \frac{\partial v}{\partial x} - \text{Kn}^2 \left[\frac{4}{3} \frac{\partial^2 \varrho}{\partial x^2} - \frac{2}{3} \frac{\partial^2 T}{\partial x^2} \right] \\ &\quad + \text{Kn}^3 \frac{2}{9} \frac{\partial^3 v}{\partial x^3} + \dots, \\ q_{CE} &= -\text{Kn} \frac{15}{4} \frac{\partial T}{\partial x} - \text{Kn}^2 \frac{7}{4} \frac{\partial^2 v}{\partial x^2} \\ &\quad - \text{Kn}^3 \left[\frac{157}{16} \frac{\partial^3 T}{\partial x^3} + \frac{5}{8} \frac{\partial^3 \varrho}{\partial x^3} \right] + \dots. \end{aligned}$$

We assume plane wave solutions of the form

$$\phi = \tilde{\phi} \exp\{i(\omega t - kx)\},$$

where $\tilde{\phi}$ is the complex amplitude of the wave, ω is its frequency, and k is its wave number. The equations can be written as

$$\mathcal{A}_{AB}(\omega, k) \tilde{u}_B = 0 \quad \text{with} \quad \tilde{u}_B = \{\tilde{\varrho}, \tilde{T}, \tilde{v}, \tilde{\sigma}, \tilde{q}\},$$

and nontrivial solutions require

$$\det[\mathcal{A}_{AB}(\omega, k)] = 0,$$

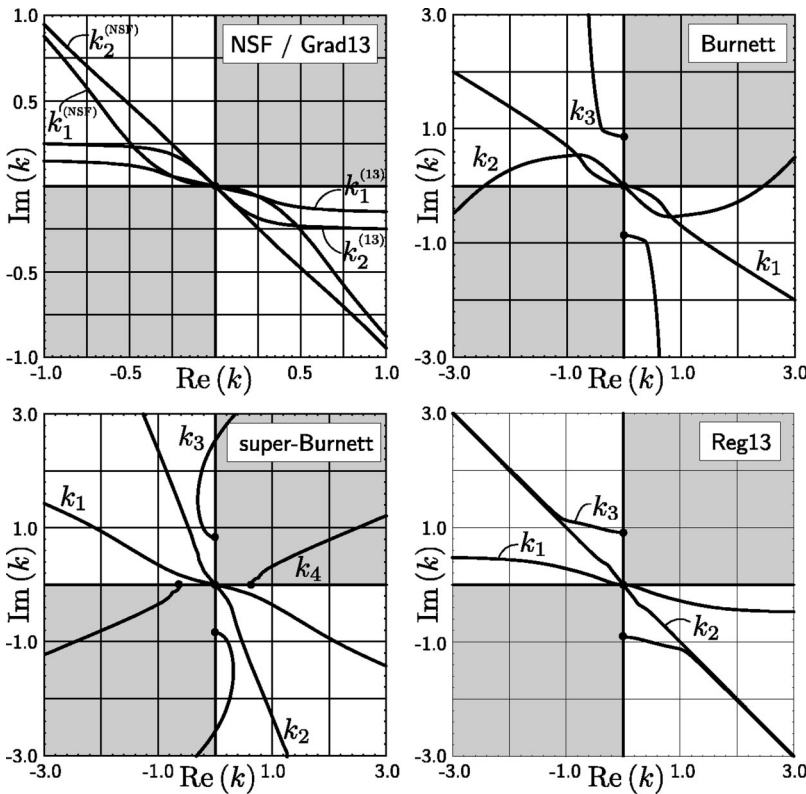


FIG. 1. The solutions $k(\omega)$ of the dispersion relation in the complex plane with ω as parameter for Navier–Stokes–Fourier, Grad’s 13 moments, Burnett, Super-Burnett, and regularized 13 moment equations. The dots denote the points where $\omega=0$.

the resulting relation between ω and k is the dispersion relation.

If a disturbance in space is considered, the wave number k is real, and the frequency is complex, $\omega = \omega_r(k) + i\omega_i(k)$. Phase velocity v_{ph} and damping α of the corresponding waves are given by

$$v_{ph} = \frac{\omega_r(k)}{k} \quad \text{and} \quad \alpha = \omega_i(k).$$

Stability requires damping, and thus $\omega_i(k) \geq 0$. It is well known that the Navier–Stokes–Fourier equations are stable, while the Burnett and Super-Burnett equations are unstable for large values of k , that is for small wavelengths.^{10,12}

If a disturbance in time at a given location is considered, the frequency ω is real, while the wave number is complex, $k = k_r(\omega) + ik_i(\omega)$. Phase velocity v_{ph} and damping α of the corresponding waves are given by

$$v_{ph} = \frac{\omega}{k_r(\omega)} \quad \text{and} \quad \alpha = -k_i(\omega).$$

For a wave traveling in positive x direction ($k_r > 0$), the damping must be negative ($k_i < 0$), while for a wave traveling in negative x direction ($k_r < 0$), the damping must be positive ($k_i > 0$).

In this section, we chose the mean free path as the reference length, and the reference time is the mean free time. Accordingly, in Eqs. (26) we have to set $\text{Kn} = 1$. It follows that the wave number is measured in units of the inverse mean free path, and the wave frequency in terms of the collision frequency $1/\tau$. Thus, the proper definition for the Knudsen number for an oscillation with frequency Ω is $\text{Kn}_\Omega = \Omega \tau$, that is $\text{Kn}_\Omega = \omega$ with the dimensionless measure

used in this section. Alternatively, for a given wave number k , we can define the proper Knudsen number as $\text{Kn}_k = k$.

B. Linear stability

We test the stability against local disturbances of frequency ω . As we have seen, stability requires different signs of real and imaginary part of $k(\omega)$. Thus, if $k(\omega)$ is plotted in the complex plane with ω as parameter, the curves should not touch the upper right nor the lower left quadrant.

Figure 1 shows the solutions for the different sets of equations considered in this paper, the dots mark the points where $\omega=0$. Grad’s 13 moment equations (Grad13), and Navier–Stokes–Fourier equations (NSF) give two different modes each, and none of the solutions violates the condition of stability (upper left in Fig. 1). This is different for the Burnett (three modes, upper right) and Super-Burnett (four modes, lower left) equations: The Burnett equations have one unstable mode, and the Super-Burnett have two unstable modes. The R13 equations, shown in the lower right, have three modes, all of them are stable.

In Fig. 2 we consider the stability against a disturbance of given wave length, or wave number k . Since it is well known that Burnett and Super-Burnett equations are unstable,¹⁰ we only show curves for the R13 equations. The figure shows the damping coefficient α and dimensionless phase velocity $c_{ph} = v_{ph}/c_0$ where $c_0 = \sqrt{(5/3)(k/m)T_0}$, or $c_0 = \sqrt{5/3}$ in dimensionless units. There are three solutions $\omega(k)$ for the dispersion relation, the “0” mode has a phase velocity of zero (not drawn). The damping coefficient is positive for all k and it follows that the R13 equations are stable.

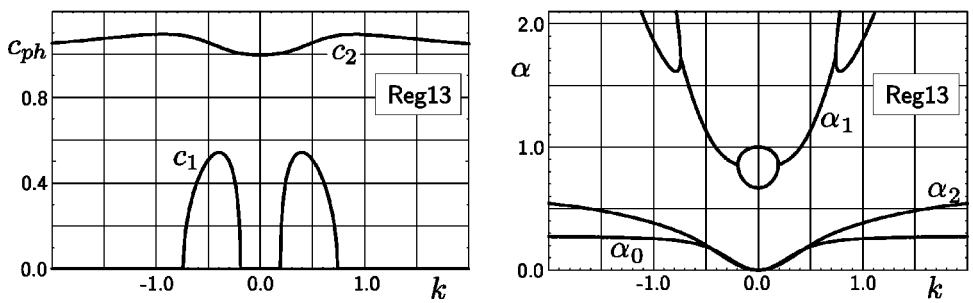


FIG. 2. Phase velocity and damping in time for the R13 equations as functions of the wave number k .

The instability of the Burnett and Super-Burnett equations is one of the major drawbacks of these theories, since it makes accurate numerical computations impossible. The R13 equations are stable for all frequencies, as well as they are stable for disturbances of any wave length. Since the main difference between R13 and (Super-) Burnett lies in the occurrence of higher order terms of order $\alpha > 3$, we conclude that these higher order terms play an important role in stabilizing the equations.

C. Dispersion and damping

We proceed by discussing the phase speeds as functions of frequency for the various methods, as depicted in Fig. 3, which shows only the positive modes. The figure shows the ratio between the phase speed and the speed of sound $c_{ph} = v_{ph}/c_0$.

All theories have one mode, denoted as c_1 with $c_1 = 1$ for small frequencies, this mode describes the propagation of sound. The mode c_2 is zero at small frequencies, and corresponds to diffusive transport of heat [there is no shear diffusion in the one-dimensional (1D) setting]. The modes c_3, c_4 in the Burnett, Super-Burnett, and R13 equations have no obvious intuitive interpretations.

At large ω (note that $\omega = Kn_\Omega = 1$ is already large in the present dimensionless description), all curves behave quite different. Most notably, the phase speeds for Grad's 13 mo-

ment equations approach constant values of 1.65 and 0.63, this reflects the hyperbolicity of the equations. The fact that the Grad 13 equations imply finite wave speeds is related to the occurrence of sub-shocks, which occur if the inflow velocity lies above the maximum wave speed.

In all theories obtained with the Chapman-Enskog expansion, the phase speeds grow monotonously with the frequency, so that signals of infinite frequency travel at infinite speeds. The corresponding damping (not shown, but see Fig. 1) is infinite as well.

The R13 equations show a mixed behavior, with two modes giving monotonous increasing phase speeds, and one mode (the sound mode) remaining finite. The R13 equations include infinite wave speeds and this is related to the fact that they give smooth shock structures for all Mach numbers, as will be shown in a future paper.

Next we ask for comparison of phase speed and damping with experiments performed by Meyer and Sessler.⁴¹ Figure 4 shows the inverse phase speed and the damping (as α/ω) as functions of the dimensionless inverse frequency $1/\omega$, computed with NSF, Grad 13, and R13 equations, and experimental data from Ref. 41. As can be seen, the R13 equations reproduce the measured values of the damping coefficient α for all dimensionless frequencies less than unity, while the NSF and Grad13 equations fail already at $\omega = 1/4$ and $\omega = 1/2$, respectively. The agreement of the R13 prediction for

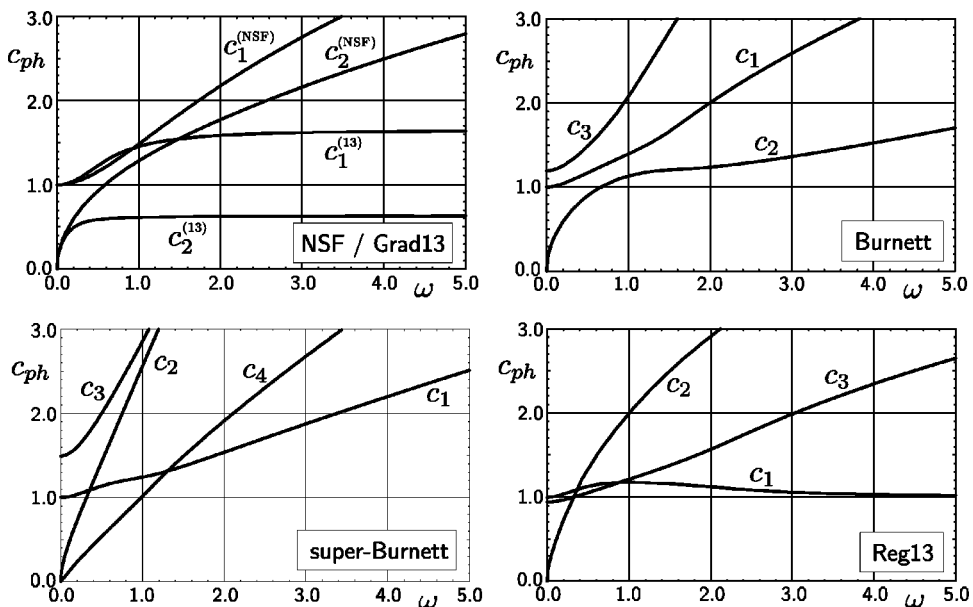


FIG. 3. Phase speed c_{ph} for the various methods as function of frequency ω .

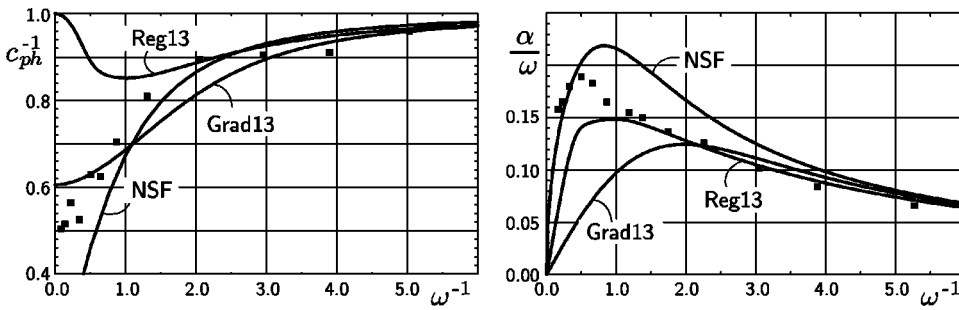


FIG. 4. Inverse phase velocity and damping, theoretical results from Navier–Stokes–Fourier, Grad’s 13 moments, and regularized 13 moments and measurements by Meyer and Sessler (Ref. 41) (dots).

the phase velocity is less striking, but also the other theories do not match well. One reason for this might be insufficient accuracy of the measurement. Altogether, the R13 equations give a remarkably good agreement with the measurements for values of $\omega < 1$.

Equations from expansions in the Knudsen number can be expected to be good only for $\text{Kn} < 1$. As we said above, the proper definition for the Knudsen number for an oscillation with dimensionless frequency ω is the frequency itself, $\text{Kn}_\Omega = \omega$. We conclude that the R13 equations allow a proper description of processes quite close to the natural limit of their validity of $\text{Kn}_\Omega = 1$. It is not surprising that all theories show discrepancies to the experiments for larger frequencies. The reasonable agreement between the NSF phase speed and experiments must be seen as coincidence.

V. KNUDSEN BOUNDARY LAYERS

In this section we briefly study boundary value problems for the linearized R13 equations. The goal is to show that the R13 equations lead to Knudsen boundary layers.

To this end we consider a simple steady state Couette flow problem: Two infinite, parallel plates move in the $\{x_2, x_3\}$ -plane with different speeds in x_2 direction. The plate distance is $L = 1$ in dimensionless units, and the plates have different temperatures. In this setting, we expect that all variables will depend only on the coordinate $x_1 = x$. Since matter cannot pass the plates, we will have $v_1 = 0$. Moreover, for symmetry reasons, there will be no fluxes in the x_3 direction, so that

$$v_i = \{0, v(x), 0\} \quad \text{and} \quad q_3 = \sigma_{13} = \sigma_{23} = 0.$$

Under these assumptions, the linearized equations (21) can be split into the flow problem with the equations

$$\frac{\partial v}{\partial x} + \frac{2}{5} \frac{\partial q_2}{\partial x} = -\frac{\sigma_{12}}{\text{Kn}} = \text{const}, \quad q_2 = \frac{9}{5} \text{Kn}^2 \frac{\partial^2 q_2}{\partial x^2},$$

and the heat transfer problem, with the equations

$$\frac{5}{2} \frac{\partial T}{\partial x} + \frac{\partial \sigma_{11}}{\partial x} = -\frac{2}{3} \frac{q_1}{\text{Kn}} = \text{const}, \quad \sigma_{11} = \frac{6}{5} \text{Kn}^2 \frac{\partial^2 \sigma_{11}}{\partial x^2}.$$

Two more nontrivial equations serve to compute ϱ , and σ_{22} , viz.

$$\sigma_{22} = \text{Kn}^2 \left[\frac{2}{3} \frac{\partial^2 \sigma_{22}}{\partial x^2} - \frac{4}{15} \frac{\partial^2 \sigma_{11}}{\partial x^2} \right], \quad \frac{\partial \varrho}{\partial x} + \frac{\partial T}{\partial x} + \frac{\partial \sigma_{11}}{\partial x} = 0.$$

The linear equations are easy to integrate, and we obtain the solution of the flow problem as

$$v(x) = v_0 - \sigma_{12} \frac{x}{\text{Kn}} - \frac{2}{5} q_2(x)$$

with

$$q_2(x) = A \sinh\left(\sqrt{\frac{5}{9}} \frac{x - \frac{1}{2}}{\text{Kn}}\right) + B \cosh\left(\sqrt{\frac{5}{9}} \frac{x - \frac{1}{2}}{\text{Kn}}\right), \quad (27)$$

where v_0, σ_{12}, A, B are constants of integration.

The solution of the heat transfer problem reads

$$T(x) = T_0 - \frac{4}{15} q_1 \frac{x}{\text{Kn}} - \frac{2}{5} \sigma_{11}(x)$$

with

$$\sigma_{11}(x) = C \sinh\left(\sqrt{\frac{5}{6}} \frac{x - \frac{1}{2}}{\text{Kn}}\right) + D \cosh\left(\sqrt{\frac{5}{6}} \frac{x - \frac{1}{2}}{\text{Kn}}\right), \quad (28)$$

where T_0, q_1, C, D are constants of integration.

Thus, in order to obtain the fields of temperature and velocity between the plates, we need eight boundary conditions. The velocities and temperatures of the two plates give only four boundary conditions, and thus additional boundary conditions are required. As of now, the problem how to prescribe meaningful boundary conditions for the R13 equations is unsolved, and we hope to be able to present proper boundary conditions (that, of course, allow for temperature jumps and velocity slips) in the future.

Nevertheless, it is worthwhile to study the general solutions (27) and (28): In the linear Navier–Stokes–Fourier case both, temperature and velocity, are straight lines according to

$$v_{\text{NSF}}(x) = v_0 - \sigma_{12} \frac{x}{\text{Kn}} \quad \text{and} \quad T_{\text{NSF}}(x) = T_0 - \frac{4}{15} q_1 \frac{x}{\text{Kn}},$$

that is for the NSF case one finds $q_2(x) = \sigma_{11}(x) = 0$.

With the R13 equations, on the other hand, these functions are nonzero as given in (27) and (28). From that, we identify $-\frac{2}{5} q_2(x)$ and $-\frac{2}{5} \sigma_{11}(x)$ as the Knudsen boundary layers for velocity and temperature according to the R13 equations. Indeed, these functions have the typical shape of a boundary layer, their largest values are found at the walls, and the curves decrease to zero within several mean free paths away from the walls.

The curves are governed by the Knudsen number, so that for small Knudsen numbers $q_2(x)$ and $\sigma_{11}(x)$ are equal to zero almost everywhere between the plates. The boundary layers are confined to a small region adjacent to the wall, and

contribute to temperature jump and velocity slip.⁴² In this case, the Navier–Stokes–Fourier theory can be used with proper jump and slip boundary conditions.

As Kn grows, the width of the boundary layers is growing as well. For Knudsen numbers above ~ 0.05 one cannot speak of boundary layers anymore, since the functions $q_2(x), \sigma_{11}(x)$ as given in (27) and (28) are nonzero anywhere in the region between the plates. In this case boundary effects have an important influence on the flow pattern.

Since, at this point, we have no recipe for prescribing all boundary values required, we cannot say whether the boundary layers obtained from the R13 equations coincide well with those of the Boltzmann equation. A recent study of heat transfer with Grad's moment equations⁴³ indicates that more moments than 26 might be needed for an accurate agreement with the Boltzmann equation. Nevertheless, results from the 26 moment case give a marked improvement when compared with the Navier–Stokes–Fourier theory, and the same can be expected from the R13 equations, which were derived from the 26 moment case.

VI. CONCLUSIONS

We presented a new set of equations for gas flows in the transition regime, termed as the regularized 13 moment equations, or R13 equations. In the present paper we have proven that the equations contain the Navier–Stokes–Fourier, Burnett and Super-Burnett equations when expanded in the appropriate order in the Knudsen number, are linearly stable for disturbances in all wavelengths or frequencies, give wave speeds and damping in good agreement with experimental data, and exhibit Knudsen boundary layers. A follow-up paper will show that the R13 equations give continuous shock structures for all Mach numbers, where shock thickness and asymmetry match well with experiments.

However, before the R13 equations can be considered as a useful tool for the computation of transitional flows, the problem of boundary values must be solved. It must be noted, though, that (Super-) Burnett equations and Grad type equations with more than 13 moments face the same problem. Some progress on solutions of boundary value problems for moment equations was reported only recently in Refs. 18, 24, 43, and 44, where the boundary conditions for the distribution function were instrumentalized in order to provide the boundary conditions for moments. We are hopeful that these studies will be helpful in understanding how a solution of the problem of boundary values for the R13 equations can be found.

Another, less important, open question is how to define the entropy for the R13 equations. It is well known that for the Burnett equations the H-theorem can be violated⁴⁵ (see Ref. 46 for a discussion), a fact that probably is related to the observed instabilities of the Burnett equations. Since the R13 system is unconditionally stable, it might well be that a proper entropy, that is with strictly non-negative entropy production, can be found. For this problem, it might be useful to compare our equations with those of Jin and Slemrod,^{16,17} which are constructed in order to guarantee a proper entropy

inequality. The study of their papers might show the road towards an entropy inequality for our equations.

Despite these open questions, the R13 equations present themselves as an interesting alternative to higher order Chapman–Enskog expansions (Burnett, Super-Burnett) and Grad's moment equations, since they combine the benefits of both methods, while avoiding their drawbacks.

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APPENDIX A: EQUATIONS FOR THE DERIVATION OF m_{ijk} , R_{ik} , AND Δ

The general moment equations for $\rho_{\langle ijk \rangle}$, $\rho_{rr\langle ik \rangle}$, and ρ_{rrss} read

$$\begin{aligned} \frac{\partial \rho_{\langle ijk \rangle}}{\partial t} + \frac{\partial \rho_{\langle ijk \rangle} v_l}{\partial x_l} + \frac{\partial \rho_{\langle ijk l \rangle}}{\partial x_l} + \frac{3}{7} \frac{\partial \rho_{rr\langle ij \rangle}}{\partial x_k} - \frac{3}{\varrho} \sigma_{\langle ij} \frac{\partial p}{\partial x_k} \\ - \frac{3}{\varrho} \sigma_{\langle ij} \frac{\partial \sigma_{kl \rangle}}{\partial x_l} + 3 \rho_{\langle l \langle ij \rangle} \frac{\partial v_k \rangle}{\partial x_l} + \frac{12}{5} q_{\langle i} \frac{\partial v_j \rangle}{\partial x_k} \\ = - \frac{3}{2} \frac{\rho_{\langle ijk \rangle}}{\tau}, \end{aligned}$$

$$\begin{aligned} \frac{\partial \rho_{rr\langle ij \rangle}}{\partial t} + \frac{\partial \rho_{rr\langle ij \rangle} v_k}{\partial x_k} + \frac{\partial \rho_{rr\langle ijk \rangle}}{\partial x_k} + \frac{2}{5} \frac{\partial \rho_{rrss\langle i}}{\partial x_j \rangle} \\ - \frac{2}{\varrho} \rho_{\langle ijr \rangle} \frac{\partial p_{rk}}{\partial x_k} - \frac{28}{5\varrho} q_{\langle i} \frac{\partial p_{jk \rangle}}{\partial x_k} + 2 \rho_{\langle ij \rangle kl} \frac{\partial v_k}{\partial x_l} \\ + 2 \rho_{rrk\langle i} \frac{\partial v_j \rangle}{\partial x_k} = - \frac{7}{6} \frac{\rho_{rr\langle ij \rangle} - \frac{k}{m} T \sigma_{ij}}{\tau}, \end{aligned}$$

$$\begin{aligned} \frac{\partial \rho_{rrss}}{\partial t} + \frac{\partial \rho_{rrss} v_k}{\partial x_k} + \frac{\partial \rho_{rrssk}}{\partial x_k} - \frac{8}{\varrho} q_j \frac{\partial p_{jk}}{\partial x_k} + 4 \rho_{rrkj} \frac{\partial v_j}{\partial x_k} \\ = - \frac{2}{3} \frac{\rho_{rrss} - 15 p^2 / \rho}{\tau}. \end{aligned}$$

The production terms on the right are computed for Maxwell molecules.

APPENDIX B: EQUATIONS FOR THE DERIVATION OF THE SUPER-BURNETT EQUATIONS

Here, we list the time derivatives of the expansion terms $\sigma_{ij}^{(1)}$, $\sigma_{ij}^{(2)}$, $q_i^{(1)}$, $q_i^{(2)}$ that are used in the computation of the Burnett and Super-Burnett equations of Sec. III. The expressions follow straight forward from eliminating time derivatives of ρ, T, v_i by means of their balance laws, which contain pressure deviator and heat flux. Since we do not go beyond the Super-Burnett order, we need only the contributions up to $\mathcal{O}(\text{Kn}^2)$ which are obtained as

$$\begin{aligned} \text{Kn} \frac{\partial \sigma_{ij}^{(1)}}{\partial t} &= 2 \text{Kn} \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j \rangle}} + 2 \text{Kn} \frac{\partial^2 T}{\partial x_{\langle i} \partial x_{j \rangle}} \\ &\quad - \frac{2}{3} \text{Kn}^2 \frac{\partial^2}{\partial x_{\langle i} \partial x_{j \rangle}} \frac{\partial v_k}{\partial x_k} - 2 \text{Kn}^2 \frac{\partial^2}{\partial x_k \partial x_k} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \\ &\quad + \mathcal{O}(\text{Kn}^3), \end{aligned} \quad (\text{B1})$$

$$\text{Kn} \frac{\partial q_i^{(1)}}{\partial t} = \frac{5}{2} \text{Kn} \frac{\partial^2 v_k}{\partial x_k \partial x_i} - \frac{75}{8} \text{Kn}^2 \frac{\partial^3 T}{\partial x_i \partial x_k \partial x_k} + \mathcal{O}(\text{Kn}^3),$$

$$\text{Kn}^2 \frac{\partial \sigma_{ij}^{(2)}}{\partial t} = \frac{4}{3} \text{Kn}^2 \frac{\partial^2}{\partial x_{\langle i} \partial x_{j \rangle}} \frac{\partial v_k}{\partial x_k} + \mathcal{O}(\text{Kn}^3), \quad (\text{B2})$$

$$\text{Kn}^2 \frac{\partial q_i^{(1)}}{\partial t} = \frac{7}{4} \text{Kn}^2 \left(\frac{\partial^3 \rho}{\partial x_i \partial x_k \partial x_k} + \frac{\partial^3 T}{\partial x_i \partial x_k \partial x_k} \right) + \mathcal{O}(\text{Kn}^3).$$

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