IMA Journal of Applied Mathematics (2011) 1−26
doi:10.1093/imamat/hxr004

Macroscopic transport models for rarefied gas flows: a brief review

HENNING STRUCHTRUP* AND PEYMAN TAHERI
Department of Mechanical Engineering, University of Victoria, Victoria BC V8W 3P6, Canada
*Corresponding author: struchtr@uvic.ca

[Received on 27 May 2010; revised on 4 September 2010; accepted on 6 September 2010]

Efficient modelling of gas microflows requires accurate, yet fast to solve, models. For finite but moderate Knudsen numbers, extended macroscopic transport equations offer an alternative to the Boltzmann equation, from which they are derived. Classical and modern approaches for the derivation of these models are reviewed, and the resulting equations are compared for their ability to describe the multitude of known rarefaction phenomena. Among the equations discussed are the Burnett and super-Burnett equations, Grad's 13 moment equations, and the regularized 13 and 26 moment equations.

Keywords: Gas microflows; regularized moment equations; Chapman–Enskog expansion.

1. Introduction

The accurate simulation of gas flows in microdevices requires effective transport models that allow for fast and accurate solutions of gas microflows. Gas flows are characterized by their Knudsen number Kn, which is defined as the ratio between the mean free path of a gas particle and the typical length scale of the flow. Classical gas flows have small Knudsen numbers, Kn $\lesssim 0.01$ (say), and can be described by the equations of classical hydrodynamics, i.e., the laws of Navier–Stokes and Fourier (NSF). For gas microflows, however, the Knudsen number is not sufficiently small to guarantee the validity of the NSF equations, and the processes must be modelled with more detailed theories. The most detailed description of gas flows is provided by the Boltzmann equation, which describes the microscopic behaviour of the gas and is valid for flows at all Knudsen numbers (Chapman & Cowling, 1970; Cercignani, 1975; Sone, 2002; Struchtrup, 2005b).

The NSF equations solve for the macroscopic quantities mass density $\rho(x_k, t)$, velocity $v_i(x_k, t)$ and temperature $T(x_k, t)$, at all locations x_k and all times t. The Boltzmann equation, on the other hand, is an equation for the particle velocity distribution $f(x_k, t, c_k)$, where c_k denotes the microscopic velocity of the particles. The interesting macroscopic quantities, e.g., ρ, v_i, T, follow from suitable averaging over the distribution function. Obviously, the NSF equations pose a mathematically less complex problem than the Boltzmann equation. Indeed, even for simple flow problems, for which NSF can be solved analytically, the Boltzmann equation must be solved numerically, either directly or by means of the direct simulation Monte Carlo method (DSMC) (Bird, 1994). Due to its complexity and stiffness codes must run for long time; in particular at intermediate Knudsen numbers in the so-called transition regime ($0.01 \leqslant$ Kn $\leqslant 10$) computational times can be measured in days or sometimes weeks.

The NSF equations can be derived from the Boltzmann equation in the limit of sufficiently small Knudsen numbers (Chapman & Cowling, 1970; Ferziger & Kaper, 1972; Kogan, 1969; Struchtrup, 2005b), and thus arises the question whether it is possible to derive macroscopic transport equations from the Boltzmann equation for flows at larger Knudsen numbers. This is indeed the case and there

are several methods to derive macroscopic equation systems that go beyond the capabilities of the NSF equations to describe rarefied gas flows. In the following, we give a brief overview over the development of this topic in recent years, with some focus on our own contributions. We shall show that, with some limitations, extended transport models are indeed able to describe rarefied gas flows with Knudsen numbers $\mathrm{Kn} \lesssim 1$ with sufficient accuracy.

For flows outside the hydrodynamic regime, that is for $\mathrm{Kn} \gtrsim 0.01$, many interesting phenomena—rarefaction effects, which do not arise in standard hydrodynamics—are found in experiments and from the analysis of the Boltzmann equation or from its numerical solution. The touchstone for any extended transport model is its capability to describe as many of these as possible. Some significant rarefaction phenomena are (a) heat flux in flow direction without temperature gradient (Baranyai *et al.*, 1992; Todd & Evans, 1995, 1997; Uribe & Garcia, 1999; Aoki *et al.*, 2002); (b) non-constant pressure profile in Couette and Poiseuille flows (Tij & Santos, 1994; Tij *et al.*, 1998; Mansour *et al.*, 1997; Uribe & Garcia, 1999; Aoki *et al.*, 2002); (c) in Poiseuille flow, the mass flow exhibits a minimum for Knudsen numbers around unity (Knudsen, 1909; Deissler, 1964; Ohwada *et al.*, 1989; Hickey & Loyalka, 1990; Lockerby *et al.*, 2004; Hadjiconstantinou, 2006), and (d) there is a characteristic dip in the temperature profile (Alaoui & Santos, 1992; Tij & Santos, 1994; Mansour *et al.*, 1997; Tij *et al.*, 1998; Aoki *et al.*, 2002; Zheng *et al.*, 2002; Xu, 2003; Xu & Li, 2004); (e) transpiration flow, that is flow induced by a temperature gradient in the wall (Sone, 2002; Sharipov & Seleznev, 1998); (f) Knudsen boundary layers at the walls (Sone, 2002; Ohwada *et al.*, 1989; Risso & Cordero, 1998); (g) phase speed and attenuation of high-frequency sound waves differ from the prediction of classical hydrodynamics (Greenspan, 1956); and (h) the detailed structure of shock waves, which cannot be reproduced by classical hydrodynamics (Alsmeyer, 1976; Gilbarg & Paolucci, 1953; Holian *et al.*, 1993).

The earliest derivation of the NSF laws from the Boltzmann equation used the Chapman–Enskog (CE) expansion to first order in the Knudsen number (Chapman & Cowling, 1970; Cercignani, 1975; Ferziger & Kaper, 1972; Kogan, 1969). While this result gave trust in the CE method, its application to higher orders gives the Burnett (Burnett, 1936) and super-Burnett equations (Shavaliyev, 1993), which turn out to be unstable in time-dependent problems (Bobylev, 1982; Rosenau, 1989; Uribe *et al.*, 2000). But even for most steady-state problems, the Burnett equations cannot be solved since they lack a complete set of boundary conditions. Moreover, the CE method, which relies on an asymptotic expansion of the Boltzmann equation in the Knudsen number, is not appropriate for Knudsen layers, and thus the Burnett and super-Burnett equations do not properly describe these. Due to these problems, attempts to stabilize the Burnett equations (Zhong *et al.*, 1993; Bobylev, 2006; Söderholm, 2007) found only limited recognition. For a detailed review of the literature on Burnett-type equations see García-Colín *et al.* (2008).

The other classical approach to extended transport equations is Grad's moment method (Grad, 1949, 1958) where the space of macroscopic variables is extended by including stress tensor σ_{ij}, heat flux vector q_i and other moments of the distribution function. The resulting equations are stable and, if the number of variables is sufficiently large, can describe Knudsen layers (Reitebuch & Weiss, 1999; Struchtrup, 2002, 2008). Nevertheless, the Grad method is not accompanied by a guideline that would state how many, and which, variables are required for flows with a given Knudsen number. While Grad provided a theory of boundary conditions for his equations (Grad, 1949), only few solutions of boundary-value problems are available in the literature (Marques & Kremer, 2001). Due to the hyperbolic character of the equations, shock structure calculations show spurious subshocks (Weiss, 1995).

In short, due to the various issues mentioned above, both, Burnett-type and Grad-type equations, do not fulfill the requirements on a macroscopic set of equations to describe rarefied gas flows.

Since 2003 we are involved in the development and evaluation of the regularized 13 moment (R13) equations which are of third order in the Knudsen number Kn, i.e., of super-Burnett order (Grad, 1958; Karlin *et al.*, 1998; Struchtrup & Torrilhon, 2003; Torrilhon & Struchtrup, 2004; Struchtrup, 2004b, 2005b). Their rational derivation from the Boltzmann equation (Struchtrup & Torrilhon, 2003; Struchtrup, 2004b, 2005b) combines elements of the CE and Grad methods with new ideas, and the equations combine the benefits of Grad and Burnett-type equations while omitting their problems.

In particular, the R13 equations are linearly stable (Struchtrup & Torrilhon, 2003; Struchtrup, 2004b, 2005b); give accurate predictions for phase speeds and damping of ultrasound waves (Struchtrup & Torrilhon, 2003; Struchtrup, 2005b); give smooth shock structures even for high-Mach numbers (Torrilhon & Struchtrup, 2004); exhibit Knudsen boundary layers (Struchtrup & Torrilhon, 2003); (Struchtrup & Thatcher, 2007a); are furnished with a complete theory of boundary conditions (Torrilhon & Struchtrup, 2008; Gu & Emerson, 2007); and obey an H-theorem for the linear case, including the boundary conditions (Struchtrup & Torrilhon, 2007b).

With this, the R13 equations currently represent the most successful extended hydrodynamic model at Burnett or super-Burnett order. They give reliable results (error below ∼5–7%) for Knudsen numbers up to Kn $\simeq$ 0.5. While the model was developed for 13 moments, all ideas (derivation, boundary conditions, numerical methods, . . .) can be applied to larger moment numbers. This extends the validity of the model to larger Knudsen numbers (Struchtrup, 2005b): Gu and Emerson have developed and solved the R26 moment equations (Gu & Emerson, 2009; Gu *et al.*, 2010) which give reliable results (error below ∼5–7%) up to Kn $\simeq$ 1.0.

A particularly important feature of the R13 and R26 equations is that they are accessible to analytical solutions of boundary-value problems, even for somewhat non-linear processes (Struchtrup & Torrilhon, 2007b, 2008; Taheri *et al.*, 2009b; Taheri & Struchtrup, 2009, 2010a,b). Moreover, suitable numerical methods allow their fast solution for steady-state problems by avoiding time stepping into equilibrium (Torrilhon & Struchtrup, 2008), which is a necessity in the DSMC method.

It should be mentioned that lattice Boltzmann schemes share some similarity with extended moment systems (Ansumali *et al.*, 2007). However, they have difficulty to describe the full array of kinematic and thermal processes and their non-linear coupling.

The text book (Struchtrup, 2005b) gives a detailed overview on background and derivation of macroscopic transport equations for rarefied gas flows. Since the book was written, a considerable amount of work on the R13, and the R26, equations was published, and the present review can be considered as an update. Nevertheless, the paper gives an complete overview on the topic. The most important results since publication of (Struchtrup, 2005b) concern boundary conditions and solutions of boundary-value problems, and we discuss some of these.

In the remainder of the paper, we first give a brief summary of basic elements of kinetic theory (Section 2), followed by a description of the derivation of Burnett, Grad and R13 equations from the Boltzmann equation (Section 3), and a summary of the theory of boundary conditions (Section 4). Finally, in Section 5, we present some analytical results to showcase rarefaction phenomena and the equations' ability—or disability—to describe these.

2. Basic kinetic theory

2.1 *Distribution function and Boltzmann equation*

We shall consider monatomic ideal gases exclusively. The basic quantity in kinetic theory is the particle distribution function $f(\mathbf{x}, t, \mathbf{c})$; $\mathbf{x}$ and t are the space and time variables, respectively, and $\mathbf{c}$ denotes the

microscopic velocities of particles. The distribution function is defined such that $f(\mathbf{x}, t, \mathbf{c})\mathrm{d}\mathbf{c}\,\mathrm{d}\mathbf{x}$ gives the number of gas particles in the phase space cell $\mathrm{d}\mathbf{c}\,\mathrm{d}\mathbf{x}$ at time t.

Macroscopic quantities are obtained by taking suitable averages, i.e., moments, of the phase density. The basic hydrodynamic variables mass density ρ, velocity v_i and internal energy u are given by

$$\rho = m\int f\,\mathrm{d}\mathbf{c}, \quad \rho v_i = m\int c_i f\,\mathrm{d}\mathbf{c}, \quad \rho u = \frac{3}{2}\rho\theta = \frac{m}{2}\int C^2 f\,\mathrm{d}\mathbf{c}. \tag{2.1}$$

Here, $\theta = \frac{k}{m}T$ is the temperature in energy units, m is the mass of a particle, k denotes Boltzmann's constant and $C_i = c_i - v_i$ is the peculiar velocity.

The pressure tensor (i.e., the negative of the stress tensor in hydrodynamics) is given by

$$p\delta_{ij} + \sigma_{ij} = m\int C_i C_j f\,\mathrm{d}\mathbf{c} \quad \text{with} \quad p = \frac{m}{3}\int C^2 f\,\mathrm{d}\mathbf{c}, \quad \sigma_{ij} = m\int C_{\langle i}C_{j\rangle} f\,\mathrm{d}\mathbf{c}, \tag{2.2}$$

where, due to $(2.1)_3$, the pressure p obeys the ideal gas law, $p = \rho\theta$, and σ_{ij} denotes what we will call the stress, that is the symmetric and tracefree part[1] of the pressure tensor, with $\sigma_{ii} = 0$, $\sigma_{ij} = \sigma_{ji}$. The heat flux vector is given by

$$q_i = \frac{m}{2}\int C^2 C_i f\,\mathrm{d}\mathbf{c}. \tag{2.3}$$

The space-time behaviour of the phase density $f(\mathbf{x}, t, \mathbf{c})$ is governed by the Boltzmann equation,

$$\frac{\partial f}{\partial t} + c_i\frac{\partial f}{\partial x_i} = \mathcal{S}. \tag{2.4}$$

Here, the two terms on the left describe the free flight of particles, and $\mathcal{S}$ on the right-hand side is the collision term which describes the change of f due to collisions among particles. The full expression for $\mathcal{S}$ can be found in the literature (Cercignani, 1975; Chapman & Cowling, 1970; Struchtrup, 2005b), here we only list its most important properties: Mass, momentum and energy are conserved in a collision, the production of entropy is always non-negative (H-theorem), in equilibrium the phase density is a Maxwellian distribution, i.e.

$$\mathcal{S} = 0 \Longrightarrow f = f_M = \frac{\rho}{m}\frac{1}{\sqrt{2\pi\theta}^3}\exp\left[-\frac{C^2}{2\theta}\right]. \tag{2.5}$$

The Boltzmann collision term $\mathcal{S}$ is a complex non-linear integral expression in f that depends also on the interaction potential between the particles. Its mathematical treatment becomes particularly simple for particles interacting with a repulsive fifth-order power potential, the so-called Maxwell molecules (Chapman & Cowling, 1970; Cercignani, 1975; Struchtrup, 2005b). More realistic potentials, e.g., general power laws, hard sphere molecules or Lennard–Jones potentials introduce higher complexity (Cercignani, 1975; Bird, 1994).

Simplified expressions for $\mathcal{S}$ which capture its basic properties are often used, the most popular of these is the Bhatnagar-Gross-Krook (BGK) model (Bhatnagar *et al.*, 1954; Struchtrup, 2005b) where

$$\mathcal{S}_{\mathrm{BGK}} = \nu(f_M - f); \tag{2.6}$$

[1]Here and in the following, indices between angular brackets denote symmetric trace-free tensors, see Ref. Struchtrup (2005b), Appendix A.2.

where ν is the average collision frequency for a particle. While the BGK model meets the above three points, it is less accurate than the Boltzmann collision term, in particular it gives a wrong value of the Prandtl number.

2.2 *Knudsen number*

Most macroscopic models for rarefied gases are derived from the Boltzmann equation by means of scaling arguments. For a proper understanding, one best considers dimensionless equations in which the Knudsen number Kn appears as the appropriate scaling parameter.

We denote the basic length scale of the problem at hand as L; this could be, e.g., the diameter of a pipe, the size of an obstacle or a wavelength. For further scaling, we use the thermal particle velocity $\bar{C} = \sqrt{2\theta}$, a reference number density n_0, and an average collision frequency ν_0. With these, we form the dimensionless quantities

$$\hat{f} = \frac{\bar{C}^3}{n_0} f, \quad \hat{x}_i = \frac{x_i}{L}, \quad \hat{t} = \frac{\bar{C}}{L} t, \quad \hat{c}_i = \frac{c_i}{\bar{C}}, \quad \hat{\mathcal{S}} = \frac{1}{\nu_0} \frac{\bar{C}^3}{n_0} \mathcal{S}; \tag{2.7}$$

the scaling of the collision term is evident from the BGK collision term (2.6).

Accordingly, the dimensionless Boltzmann equation reads

$$\frac{\partial \hat{f}}{\partial \hat{t}} + \hat{c}_i \frac{\partial \hat{f}}{\partial \hat{x}_i} = \frac{1}{\mathrm{Kn}} \hat{\mathcal{S}}(f, f). \tag{2.8}$$

with the Knudsen number

$$\mathrm{Kn} = \frac{1/\nu_0}{L/\bar{C}} = \frac{\lambda}{L}.$$

Here, $\lambda = \bar{C}/\nu_0$ is the mean free path of a particle, that is, the average distance a particle travels between two collisions; the Knudsen number is the ratio between mean free path and macroscopic length scale L. One distinguishes the following regimes for processes, with the appropriate transport equations:

- $\mathrm{Kn} \lesssim 0.01$: Hydrodynamic regime, NSF equations.
- $0.01 \lesssim \mathrm{Kn} \lesssim 0.1$: Slip flow regime, NSF with jump and slip boundary conditions
- $0.1 \lesssim \mathrm{Kn} \lesssim 10$: Transition regime, Boltzmann equation or extended macroscopic models
- $\mathrm{Kn} \gtrsim 10$: Free molecular flow, Boltzmann equation.

As will become clear in the next section, processes with very small Knudsen numbers can be described by the classical transport equations. For relatively small Knudsen numbers in the slip-flow regime it suffices to provide appropriate boundary conditions to the NSF equation. All flows with Knudsen numbers above 0.1 (say), are rarefied flows, and must be described with extended macroscopic models or the Boltzmann equation.

For small mean free path—and Knudsen number—the gas particles travel only a short distance, and carry momentum and energy only to their immediate neighbourhood. Thus, transport processes are essentially local. When the mean free path—and thus the Knudsen number—becomes comparatively large, the gas particles travel larger distances between collisions, and carry energy and momentum to more distant locations: transport processes become non-local. Capturing non-local effects with continuum models requires higher-order gradients in the transport laws, as will be seen in the Burnett-type equations, or extended sets of equations of balance law-type, as will be seen for moment equations.

2.3 *Macroscopic equations*

For many processes, the main interest is not the detailed knowledge of the distribution function f, but the knowledge of its macroscopically meaningful moments, in particular density, velocity, temperature, shear stress and heat flux. These can be obtained by solving the Boltzmann equation for f and subsequent integration. An alternative to this is to construct, and solve, a set of equations for the macroscopic quantities $\{\rho, v_i, \theta, \ldots\}$.

Multiplication of the Boltzmann equation (2.4) with $\left\{m, mc_i, \frac{m}{2}C^2\right\}$ and subsequent integration over the microscopic velocity yields the conservation laws for mass, momentum and internal energy,

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} &= 0, \\ \rho \frac{\partial v_i}{\partial t} + \rho v_k \frac{\partial v_i}{\partial x_k} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} &= 0, \\ \frac{3}{2}\rho \frac{\partial \theta}{\partial t} + \frac{3}{2}\rho v_k \frac{\partial \theta}{\partial x_k} + \frac{\partial q_k}{\partial x_k} &= -(p\delta_{ij} + \sigma_{ij})\frac{\partial v_i}{\partial x_j}. \end{aligned} \tag{2.9}$$

Multiplication of the Boltzmann equation with $-k \ln \frac{f}{y}$ (y is a constant) yields the balance of entropy, which has a non-negative production. For space reasons, we shall not further discuss it, see Cercignani (1975), Chapman & Cowling (1970) and Struchtrup (2005b) for details.

The conservation laws (2.9) together with the definitions for stress and heat flux (2.2, 2.3) are exact, that is they are valid for any solution f of the Boltzmann equation. To guarantee the proper physics, the five conservation laws must be among the equations considered to describe the gas on the macroscopic level. Obviously, since they contain stress σ_{ij} and heat flux q_i, the conservation laws alone do not form a closed set of equations for the hydrodynamic variables $\{\rho, v_i, \theta\}$; additional equations for σ_{ij} and q_i are required.

The idea of macroscopic continuum approximations is to close the set of equations by deriving additional macroscopic equations for σ_{ij} and q_i from the Boltzmann equation through rational approximation procedures. Various methods are available to this end, and the corresponding additional equations for σ_{ij} and q_i, will be discussed in the sequel.

3. Transport equations

3.1 *Chapman-Enskog method*

The best known approach to derive macroscopic transport equations from the Boltzmann equation is the CE method (Cercignani, 1975; Chapman & Cowling, 1970; Kogan, 1969; Ferziger & Kaper, 1972; Struchtrup, 2005b), which is based on the dimensionless form of the Boltzmann equation (2.8). To simplify notation, we will not write the hats that denote dimensionless quantities.

In the limit $\mathrm{Kn} \to 0$, the collision term $\mathcal{S}$ must vanish, and it follows from the properties listed in Section 2 that the corresponding phase density is the local Maxwellian (2.5), $f^{(0)} = f_M$. Evaluation of σ_{ij} and q_i with the Maxwellian gives zero stress and heat flux,

$$\sigma_{ij}^{(0)} = q_i^{(0)} = 0. \tag{3.1}$$

Insertion of this into the conservation laws (2.9) yields the Euler equations, which form the appropriate set of transport equations for flows with negligible Knudsen numbers. Note that the Euler equations do not describe dissipative processes, viscosity and heat conductivity are effectively zero.

The idea of the CE expansion method is to add corrections to the local equilibrium distribution by adding terms of higher orders in the Knudsen number,

$$f = f^{(0)} + \mathrm{Kn} f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \cdots, \tag{3.2}$$

subject to the condition that the hydrodynamic variables $\{\rho, v_i, \theta\}$ are the same at any level of expansion, so that

$$\rho \left\{1, v_i, \frac{3}{2}\theta\right\} = m \int \left\{1, c_i, \frac{C^2}{2}\right\} f^{(0)} \mathrm{d}\mathbf{c}, \quad 0 = \int \left\{1, c_i, \frac{C^2}{2}\right\} f^{(\alpha)} \mathrm{d}\mathbf{c} (\alpha \geqslant 1). \tag{3.3}$$

The above compatibility conditions guarantee that only the equations for the non-equilibrium variables σ_{ij} and q_i change with increasing degree of approximation,

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \mathrm{Kn}\sigma_{ij}^{(1)} + \mathrm{Kn}^2\sigma_{ij}^{(2)} + \cdots, \quad q_i = q_i^{(0)} + \mathrm{Kn}q_i^{(1)} + \mathrm{Kn}^2 q_i^{(2)} + \cdots. \tag{3.4}$$

The expansion parameters $f^{(\alpha)}$ are determined successively, by plugging the series (3.2) into the Boltzmann equation, and equating terms with the same factors in powers of the Knudsen number. This leads to an iterative structure, where the correction at order α is a function of (derivatives of) the lower-order corrections, $f^{(\alpha)} = \mathcal{F}(f^{(\beta)}, 0 \leqslant \beta < \alpha)$, see, e.g., Kogan (1969) and Struchtrup (2005b). All correction terms depend only on the hydrodynamic variables and their gradients,[2] since the zeroth-order term—the Maxwellian—depends only on the hydrodynamic variables $\{\rho, v_i, \theta\}$. Stress and heat flux are computed from the approximation (3.2) by accounting for terms up to a certain order, and the resulting expressions will relate σ_{ij} and q_i to the hydrodynamic variables and their gradients.

We have already seen that to zeroth order, the expansion yields the Euler equations (3.1). The first-order correction gives the laws of NSF,

$$\sigma_{ij}^{(1)} = -2\mu \frac{\partial v_{\langle i}}{\partial v_{j\rangle}}, \quad q_i^{(1)} = -\kappa \frac{\partial \theta}{\partial x_i}. \tag{3.5}$$

The most important success of the CE method is that it gives accurate expressions for viscosity μ and heat conductivity κ, which relate these to the microscopic interaction potential and the hydrodynamic variables (Kogan, 1969; Struchtrup, 2005b). In particular one finds, in accordance with experiments, that the viscosity depends only on temperature and not on density. For power potentials, the CE method yields

$$\mu = \mu_0 \left(\frac{\theta}{\theta_0}\right)^{\omega} \tag{3.6}$$

with $\omega = 1/2$ for hard spheres and $\omega = 1$ for Maxwell molecules; experiments indicate $\omega \simeq 0.8$ for argon (Bird, 1994). Heat conductivity and viscosity are related through the Prandtl number,[3]

$$\mathrm{Pr} = \frac{5}{2}\frac{\mu}{\kappa} \simeq \frac{2}{3}.$$

[2]Time derivatives are replaced by means of the conservation laws (Kogan, 1969; Struchtrup, 2005b).

[3]Our defintion of the Prandtl number differs from the usual one by a factor $\frac{k}{m}$ due to the use of θ instead of T.

The value of Pr varies only slightly (less than 1%) with the molecule model, and measured values are close to 0.66 (Chapman & Cowling, 1970). The BGK model relates viscosity and heat conductivity to collision frequency as $\mu_{\rm BGK} = \frac{p}{\nu}$, and $\kappa = \frac{5}{2}\frac{p}{\nu}$, so that $\mathrm{Pr}_{\rm BGK} = 1$.

For larger Knudsen numbers, i.e., for rarefied flows, higher-order terms must be considered in the CE expansion. Including second order in Kn results in the Burnett equations (Burnett, 1936; Chapman & Cowling, 1970; Kogan, 1969; Struchtrup, 2005b),

$$\sigma_{ij}^{(2)} = \frac{\mu^2}{p}\left[\frac{10}{3}\frac{\partial v_k}{\partial x_k}S_{ij} - 2\left(\frac{\partial}{\partial x_{\langle i}}\left(\frac{1}{\rho}\frac{\partial p}{\partial x_{j\rangle}}\right) + \frac{\partial v_k}{\partial x_{\langle i}}\frac{\partial v_{j\rangle}}{\partial x_k} + 2\frac{\partial v_k}{\partial x_{\langle i}}S_{j\rangle k}\right)\right.$$
$$\left. +3\frac{\partial^2\theta}{\partial x_{\langle i}\partial x_{j\rangle}} + 0\frac{\partial\theta}{\partial x_{\langle i}}\frac{\partial \ln p}{\partial x_{j\rangle}} + 3\frac{1}{\theta}\frac{\partial\theta}{\partial x_{\langle i}}\frac{\partial\theta}{\partial x_{j\rangle}} + 8S_{k\langle i}S_{j\rangle k}\right], \tag{3.7}$$

$$q_i^{(2)} = \frac{\mu^2}{\rho}\left[\frac{75}{8}\frac{\partial v_k}{\partial x_k}\frac{\partial \ln\theta}{\partial x_i} - \frac{45}{8}\left(\frac{2}{3}\frac{\partial^2 v_k}{\partial x_k\partial x_i} + \frac{2}{3}\frac{\partial v_k}{\partial x_k}\frac{\partial \ln\theta}{\partial x_i} + 2\frac{\partial v_k}{\partial x_i}\frac{\partial \ln\theta}{\partial x_k}\right)\right.$$
$$\left. -3S_{ik}\frac{\partial \ln p}{\partial x_k} + 3\frac{\partial S_{ik}}{\partial x_k} + 3\frac{39}{4}S_{ik}\frac{\partial \ln\theta}{\partial x_k}\right], \tag{3.8}$$

with the abbreviation $S_{ij} = \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$. The many coefficients appearing in the Burnett equations depend on details of the intermolecular interaction that manifests itself in the collision term $\mathcal{S}$. The above equations are valid for Maxwell molecules, see Reinecke & Kremer (1990) for the appropriate coefficients for other molecular interaction potentials.

The third-order CE expansion yields the super-Burnett equations. Their computation is extremely cumbersome, and to our knowledge the full 3D non-linear super-Burnett equations were never derived. One only finds the linearized equations in 3D (Shavaliyev, 1993; Bobylev, 1982; Struchtrup & Torrilhon, 2003), and the non-linear equations for 1D geometry (Shavaliyev, 1993; Fiscko & Chapman, 1989; Torrilhon & Struchtrup, 2004).

The equations of NSF cease to be accurate for Knudsen numbers above $\sim$ 0.01, and one would expect 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 (Bobylev, 1982; Rosenau, 1989; Torrilhon & Struchtrup, 2004), and they lead to unphysical oscillations in steady-state processes (Struchtrup, 2005a), and thus cannot be used in numerical simulations.

Zhong *et al.* (1993) suggested the 'augmented Burnett equations' where some terms of super-Burnett order (but not the actual super-Burnett terms) are added to the Burnett equations to stabilize these. This approach lacks a rational derivation from the Boltzmann equation (Torrilhon & Struchtrup, 2004).

For reference in subsequent sections, we print the distribution function for the NSF equations

$$f_{|CE} = f_M\left[1 + \frac{\sigma_{ik}^{(1)}}{2p}\frac{C_{\langle i}C_{k\rangle}}{\theta} + \frac{2}{5}\frac{q_k^{(1)}}{p\theta}C_k\left(\frac{C^2}{2\theta} - \frac{5}{2}\right)\right]. \tag{3.9}$$

3.2 *Grad moment method*

Grad suggested an alternative approach in which the number of variables is extended beyond the five hydrodynamic variables ρ, v_i, θ, by adding stress σ_{ij}, heat flux q_i and other moments to the list of

variables (Grad, 1949, 1958). Just like the conservation laws, the transport equations for the additional variables are obtained by taking moments of the Boltzmann equation. And again, due to the occurrence of moments which are not among the variables, the resulting set of equations does not form a closed set for the chosen variables and thus requires a closure argument. For this, Grad suggests to approximate the phase density by an expansion f_G in Hermite polynomials about the equilibrium distribution (the local Maxwellian), where the expansion coefficients are related to the moments (Grad, 1949, 1958).

A crucial point in the method is the question which, and how many, moments are needed to describe a process. Grad's method does not provide an argument that links the Knudsen number to the set of moments to be considered as variables. In general, experience shows that the number of moments must be increased with increasing Knudsen number (Müller & Ruggeri, 1998; Struchtrup, 2002; Weiss, 1995; Au *et al.*, 2001; Struchtrup, 2008).

If one considers only the hydrodynamics variables $\{\rho, v_i, \theta\}$, the Grad method gives the Euler equations, which do not include dissipation and are valid only for $\mathrm{Kn} \to 0$.

To include dissipation, at least stress and heat flux must be considered as well—this gives the best known set of Grad-type moment equations, the 13 moment system with the variables $\{\rho, v_i, \theta, \sigma_{ij}, q_i\}$. The corresponding moment equations are obtained by multiplying the Boltzmann equation with $\left\{m, mc_i, \frac{m}{2}C^2, \; mC_{\langle i}C_{j\rangle}, \frac{m}{2}C^2C_i\right\}$. This gives the conservation laws (2.9) plus additional moment equations for stress and heat flux,

$$\frac{\partial \sigma_{ij}}{\partial t} + v_k\frac{\partial \sigma_{ij}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2p\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k} = \mathcal{P}_{ij}, \tag{3.10}$$

$$\begin{aligned}\frac{\partial q_i}{\partial t} &+ v_k\frac{\partial q_i}{\partial x_k} + \frac{5}{2}p\frac{\partial \theta}{\partial x_i} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} - \theta\sigma_{ik}\frac{\partial \ln\rho}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\\ &+ \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{1}{2}\frac{\partial R_{ik}}{\partial x_k} + \frac{1}{6}\frac{\partial \Delta}{\partial x_i} + m_{ijk}\frac{\partial v_j}{\partial x_k} - \frac{\sigma_{ij}}{\rho}\frac{\partial \sigma_{jk}}{\partial x_k} = \mathcal{P}_i.\end{aligned} \tag{3.11}$$

Equations (3.10) and (3.11) contain additional moments of the distribution function, which are defined as

$$\Delta = m\int C^4(f - f_M)\mathrm{d}\mathbf{c}, \quad R_{ij} = m\int (C^2 - 7\theta)C_{\langle i}C_{j\rangle}\, f\, \mathrm{d}\mathbf{c}, \quad m_{ijk} = m\int C_{\langle i}C_jC_{k\rangle}\, f\, \mathrm{d}\mathbf{c}. \tag{3.12}$$

The terms on the right-hand sides are the moments of the Boltzmann collision term,

$$\mathcal{P}_{ij} = m\int C_{\langle i}C_{j\rangle}\mathcal{S}\, \mathrm{d}\mathbf{c}, \quad \mathcal{P}_i = \frac{m}{2}\int C^2C_i\mathcal{S}\, \mathrm{d}\mathbf{c}. \tag{3.13}$$

Obviously, the set of equations can be closed by finding expressions for $\Delta, R_{ij}, m_{ijk}, \mathcal{P}_{ij}, \mathcal{P}_i$ that relate these to the basic 13 variables $\{\rho, v_i, \theta, \sigma_{ij}, q_i\}$. To this end, the Grad method provides the distribution Grad (1949, 1958); Struchtrup (2005b)

$$f_{|13} = f_M\left[1 + \frac{\sigma_{ik}}{2p}\frac{C_{\langle i}C_{k\rangle}}{\theta} + \frac{2}{5}\frac{q_k}{p\theta}C_k\left(\frac{C^2}{2\theta} - \frac{5}{2}\right)\right]. \tag{3.14}$$

By comparing the distribution functions (3.9) and (3.14), it becomes evident that they are quite similar. However, the first-order CE, phase density contains only the first approximations to stress and heat flux,

$\sigma_{ij}^{(1)}$ and $q_i^{(1)}$, while the Grad distribution contains both as independent variables, σ_{ij} and q_i, which are to be determined from the moment equations (3.10) and (3.11).

The function (3.14) recovers the basic 13 variables and allows to compute the unknowns (3.12) and (3.13) as

$$\Delta = R_{ij} = m_{ijk} = 0, \quad \mathcal{P}_{ij} = -\frac{p}{\mu}\sigma_{ij}, \quad \mathcal{P}_i = -\frac{2}{3}\frac{p}{\mu}q_i. \tag{3.15}$$

Insertion of (3.15) into (3.10) and (3.11) gives, together with (2.9), the closed set of equations for the 13 variables.

The Grad 13 equations have two major drawbacks: (a) The equations are symmetric hyperbolic for most values of the variables, and this leads to shock structures with discontinuities (subshocks) for Mach numbers above 1.65 (Müller & Ruggeri, 1998; Weiss, 1995). (b) Since Grad's method is not linked to the Knudsen number, the range of applicability for the equations is unclear.

These problems remain for Grad-type equations with more variables, which give smooth shocks up to higher, but not too high, Mach numbers (Weiss, 1995). The 13 moment equations do not describe Knudsen boundary layers (Struchtrup, 2003b, 2002), however, increasing the number of moments allows to compute these (Reitebuch & Weiss, 1999; Struchtrup, 2002, 2003a).

For large Mach or Knudsen numbers, one has to face hundreds of moment equations for which computations are only manageable for simple geometries (Weiss, 1990; Müller & Ruggeri, 1998; Struchtrup, 2002). Indeed, the goal of a macroscopic set of equations must be to have a simplification compared to the Boltzmann equation and using hundreds of moments does not achieve this goal.

Grad moment equations do not posses an entropy. Several variants of the moment method were suggested in the past to correct for this deficiency. The closure by maximization of entropy (Müller & Ruggeri, 1998; Dreyer, 1987; Levermore, 1996) leads to severe problems in detail (Junk, 1998, 2003; Dreyer *et al.*, 2001) and cannot provide an explicit closure. Just recently, a set of 13 moment equations with entropy was suggested by Öttinger (2010a). Solutions to these equations are under development, and one must wait for these for a proper assessment, see Struchtrup & Torrilhon (2010) and Öttinger (2010b) for preliminary comment.

3.3 *Combining the Chapman-Enskog and Grad methods*

Equation (3.4) shows that the CE expansion gives stress and heat flux in terms of the Knudsen number; higher moments can be expanded similarly. Thus, one can apply the CE expansion on moment equations by expanding the non-equilibrium moments in Kn. Reinecke and Kremer extracted the NSF and Burnett equations from extended Grad-type moment systems (Reinecke & Kremer, 1990, 1996). In the original CE method, one first expands, and then integrates the resulting distribution function to compute its moments. In the Reinecke–Kremer–Grad method, the order of integration and expansion is exchanged.

For Maxwell molecules, Knudsen number expansion of the Grad 13 moment equations yields the NSF equations at first order, and the Burnett equations at second order. The super-Burnett equations result from the third-order CE expansion of the 26 moment set (which adds Δ, R_{ij}, m_{ijk} to the list of variables) (Struchtrup, 2003b; Struchtrup & Torrilhon, 2003; Torrilhon & Struchtrup, 2004; Struchtrup, 2005b).

While the Reinecke–Kremer–Grad method does not give new results, it allows for an easier access to higher-order CE expansions, in particular, the Burnett equations. The method does not solve the stability problems of the Burnett and super-Burnett equations.

The Grad equations, on the other hand, are stable, and, as the Reinecke–Kremer–Grad method shows, they contain higher-order contributions in the Knudsen number. Naturally, the question arises whether CE-like scaling can be used to relate sets of moment equations to Knudsen number.

Struchtrup and Torrilhon considered the Grad 26 moment system and assumed different time scales for the 13 basic variables of the 13 moment equations on one side, and all higher moments on the other (Struchtrup & Torrilhon, 2003; Torrilhon & Struchtrup, 2004; Struchtrup, 2005b). Only the latter are expanded in the Knudsen number with the CE method. Effectively, this method—first suggested as a side note in Grad (1958)—relies on an expansion about a non-equilibrium state which is defined through the 13 variables. This gives a correction to the Grad 13 equations, the R13 moment equations.

A similar idea was used earlier in Karlin *et al.* (1998) for the linearized Boltzmann equation. They compute an approximation to the distribution function, which is used to derive a set of linear equations for the 13 moments. Their equations have the same structure as the linearized R13 equations; however, they did not determine the numerical values of the various coefficients.

The time scale splitting used in these arguments is somewhat artificial since in reality, all moments change on similar time scales, which are of the order of the mean collision frequency. Thus, an alternative approach to the problem was developed in Struchtrup (2004a,b, 2005b), partly based on earlier work by Müller *et al.* (2003).

The *order of magnitude method* considers the infinite coupled set of *all* possible moment equations. The CE expansion is used only to establish the Knudsen number order of the moments: The moments ϕ are expanded according to

$$\phi = \phi_0 + \mathrm{Kn}\phi_1 + \mathrm{Kn}^2\phi_2 + \mathrm{Kn}^3\phi_3 + \cdots ,$$

and their leading order is determined by inserting this ansatz into the complete set of moment equations. A moment is said to be of leading order γ if $\phi_\beta = 0$ for all $\beta < \gamma$. After the order of all moments is established, new variables are constructed by linear combination such that the number of moments at a given order γ is minimal. This step does not only simplify the later discussion, but gives an unambiguous set of moments at order γ. Finally, a set of equations is said to be accurate of order γ_0, when stress σ_{ij} and heat flux q_i are known within the order $\mathrm{O}(\mathrm{Kn}^{\gamma_0})$. The appropriate set of equations at order γ_0 includes only those terms in all equations whose leading order of *influence* in the conservation laws is $\gamma \leqslant \gamma_0$. Luckily, in order to evaluate this condition, it suffices to start with the conservation laws, and step by step, order by order, add the relevant terms that are required (Struchtrup, 2004a,b, 2005b).

The order of magnitude method was applied to Maxwell molecules in Struchtrup (2004b, 2005b). It yields the Euler equations at zeroth order, the NSF equations at first order and Grad's 13 moment equations $\left(\text{with omission of the non-linear term } \frac{\sigma_{ij}}{\rho}\frac{\partial \sigma_{jk}}{\partial x_k}\right)$ at second order. The regularized 13 moment equations (R13) are obtained as the third-order approximation, they consist of the conservation laws (2.9) and the balance laws for stress (3.10) and heat flux (3.11) which now are closed by the expressions[4]

$$\Delta = -\frac{\sigma_{ij}\sigma_{ij}}{\rho} - 12\frac{\mu}{p}\left[\theta\frac{\partial q_k}{\partial x_k} + \theta\sigma_{kl}\frac{\partial v_k}{\partial x_l} + \frac{7}{2}q_k\frac{\partial \theta}{\partial x_k} - \underline{q_k\frac{\theta}{p}\frac{\partial p}{\partial x_k}}\right],$$

[4]There are some differences between the original R13 equations of Struchtrup & Torrilhon (2003) and the equations presented here, which result from the order of magnitude method. The original equations contain some higher (fourth-) order terms, and were derived for the linearized collision operator, see Struchtrup (2005b) for details and discussion.

$$R_{ij} = -\frac{4}{7}\frac{1}{\rho}\sigma_{k\langle i}\sigma_{j\rangle k} - \frac{24}{5}\frac{\mu}{p}\left[\theta\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2q_{\langle i}\frac{\partial\theta}{\partial x_{j\rangle}} + \frac{10}{7}\theta\sigma_{k\langle i}\frac{\partial v_{\langle j\rangle}}{\partial x_{k\rangle}} - \underline{\frac{\theta}{p}q_{\langle i}\frac{\partial p}{\partial x_{j\rangle}}}\right]$$

$$m_{ijk} = -2\frac{\mu}{p}\left[\theta\frac{\partial\sigma_{\langle ij}}{\partial x_{k\rangle}} + \sigma_{\langle ij}\frac{\partial\theta}{\partial x_{k\rangle}} + \frac{4}{5}q_{\langle i}\frac{\partial v_{j}}{\partial x_{k\rangle}} - \underline{\sigma_{\langle ij}\frac{\theta}{p}\frac{\partial p}{\partial x_{k\rangle}}}\right]. \tag{3.16}$$

The moments of the collision operator $(3.15)_{2,3}$ are exact for Maxwell molecules, and remain unchanged, $\mathcal{P}_{ij} = -\frac{p}{\mu}\sigma_{ij}$, $\mathcal{P}_i = -\frac{2}{3}\frac{p}{\mu}q_i$. The appropriate phase density for the R13 equations is Grad's phase density for 26 moments, where the higher moments are replaced by the constitutive relations (3.16).

A closer inspection of the regularized equations (3.16) shows that the terms added to the original Grad 13 moment equations are of super-Burnett order. Accordingly, the CE expansion of the R13 equations reproduces the results of the CE expansion of the Boltzmann equation up to super-Burnett order (Struchtrup & Torrilhon, 2003).

The scaled and dimensionless balance of momentum can be written as $\frac{\partial\hat{p}}{\partial\hat{x}_i} = -\mathrm{M}\hat{\rho}\frac{\partial\hat{v}_i}{\partial\hat{t}} - \mathrm{M}^2\hat{\rho}\hat{v}_k\frac{\partial\hat{v}_i}{\partial\hat{x}_k} - \mathrm{Kn}\frac{\partial\hat{\sigma}_{ik}}{\partial\hat{x}_k}$. Thus, for processes with sufficiently small Mach numbers ($\mathrm{M} \leqslant \mathrm{Kn}$, or, for steady flows, $\mathrm{M}^2 \leqslant \mathrm{Kn}$), the pressure gradient is of order O(Kn). It follows that the underlined non-linear terms in (3.16) contribute above the super-Burnett order and must be removed. Indeed, would these terms be kept, additional boundary conditions were required for the solution of the equations (Torrilhon & Struchtrup, 2008).

For general, i.e., non-Maxwellian, molecule types the order of magnitude method was performed up to second order in Struchtrup (2004a, 2005b). The resulting equations are a generalization of Grad's 13 moment equations, where all terms have coefficients which are related to the Burnett coefficients. The CE expansion to second order gives the Burnett equations with the proper Burnett coefficients.

For the linearized R13 equations, an entropy inequality was found for the linearized equations (Struchtrup & Torrilhon, 2007b), which also includes boundaries.

Jin & Slemrod (2001) and Jin *et al.* (2002) proposed an alternative regularization by constructing a set of equations that gives the Burnett equations in a second-order CE expansion and gives a positive entropy production for all values of the variables. Up to second order, their equations agree with the generalized Grad 13 equations to which they add terms of super-Burnett order that were designed to achieve their goal. These higher-order terms cannot be justified from the Boltzmann equation (Struchtrup, 2005b).

The R13 equations give smooth shock structures for high Mach numbers, and they are stable. Therefore, this combination of the CE and Grad methods yields a marked improvement over the original methods.

4. Boundary conditions

4.1 *How many boundary conditions are required?*

For the solution of boundary-value problems, all sets of macroscopic equations, NSF, Burnett and super-Burnett, Grad, or R13 equations, must be furnished with an appropriate set of boundary conditions. Before we show how to obtain boundary conditions for the transport equations, we ask how many boundary conditions are actually required for their solution. A detailed discussion and evaluation of the ideas summarized below is found in Torrilhon & Struchtrup (2008).

NSF equations, Grad moment equations and regularized moment equations can all be written as a first-order system. In compact notation,

$$\mathcal{B}_{AB}\frac{\partial u_B}{\partial t} + \mathcal{A}^k_{AB}\frac{\partial u_B}{\partial x_k} = \mathcal{P}_A,$$

where $\mathcal{A}^k_{AB}$, $\mathcal{B}_{AB}$ and $\mathcal{P}_A$ are functions of the variables u_A. For instance, in the R13 equations $u_A = \{\rho, v_i, \theta, \sigma_{ij}, q_i, m_{ijk}, \Delta, R_{ij}\}$, and the matrix $\mathcal{B}_{AB}$ is diagonal, with value zero for $\{m_{ijk}, \Delta, R_{ij}\}$.

We have not tried to bring the Burnett and super-Burnett equations into the same form, therefore we cannot say whether for these the matrices depend only on the variables of the first-order system (u_A) or whether they also depend on the derivatives of the u_A.

The number of initial and boundary equations required is equal to the number of integrations one has to perform with respect to time or space variables. Therefore, the number of initial conditions required is equal to the number of non-zero eigenvalues of $\mathcal{B}_{AB}$, which equals the number of non-zero diagonal elements, and thus the number of primary variables, e.g., $\{\rho, v_i, \theta, \sigma_{ij}, q_i\}$ for R13.

Correspondingly, the number of non-zero eigenvalues of the matrices $\mathcal{A}^k_{AB}$ equals the number of boundary conditions required for boundaries with normal pointing into direction k. Since $\mathcal{A}^k_{AB}$ depends on the u_A, this number can depend on the flow conditions. For flows with conditions such that the underlined pressure gradient terms in the R13 equations (3.16) can be ignored, the boundary conditions given below will suffice.

4.2 *Microscopic boundary condition*

Since the macroscopic transport equations are derived from the Boltzmann equation, it is natural to base the derivation of their boundary conditions on the boundary condition for the Boltzmann equation.

For the discussion, we consider Maxwell's well-known wall boundary condition, where the fraction $(1-\chi)$ of incident particles is reflected elastically, and the remaining fraction χ is thermalized, that is, leaves the wall in a Maxwellian governed by wall velocity v_i^W and wall temperature θ_W (Cercignani, 1975; Struchtrup, 2005b); χ is the accommodation coefficient. With the particle velocity in the rest frame of the wall denoted by $C_k^W = c_i - v_i^W$, Maxwell's boundary condition reads

$$\bar{f} = \begin{cases} \chi f_W + (1-\chi)\tilde{f}_G, & C_k^W n_k \geqslant 0 \\ f_G, & C_k^W n_k \leqslant 0. \end{cases} \tag{4.1}$$

Here, f_G denotes the distribution function of the gas, which is also the distribution of incident particles, n_k is the wall normal, $\tilde{f}_G = f_G(C_k^W - 2C_j^W n_j n_k)$ is the distribution of the specularly reflected particles (inverted normal velocity component), and f_W is the wall Maxwellian,

$$f_W = \frac{\rho_W}{m}\sqrt{\frac{1}{2\pi\theta_W}}^3 \exp\left[-\frac{C_W^2}{2\theta_W}\right]. \tag{4.2}$$

The density ρ_W has to be determined such that the wall does not accumulate particles, i.e., from

$$\int_{C_k^W n_k \leqslant 0} C_k^W n_k \bar{f}\, \mathrm{d}\mathbf{c} = -\int_{C_k^W n_k \geqslant 0} C_k^W n_k \bar{f}\, d\mathbf{c}.$$

The slip velocity $V_i = v_i - v_i^W$ is parallel to the wall, $V_k n_k = 0$. Therefore, particle velocity c_i, particle velocity relative to the wall C_i^W, and peculiar velocity C_i are related as

$$C_i^W = c_i - v_i^W = C_i + V_i, \quad C_i^W n_i = C_i n_i. \tag{4.3}$$

4.3 *Boundary conditions for moments*

Boundary conditions for moments are constructed as follows: we write the moments as $u_A = \int \Psi_A f d\mathbf{c}$, where $\Psi_A(c_k)$ denotes the moment generating tensor polynomials in c_k with a suitable multi-index A. The flux of the moment u_A is $F_{Ak} = \int \Psi_A c_k f \, \mathrm{d}\mathbf{c}$. For an observer resting with the wall, who observes the particle velocity C_i^W, the normal flux computed with the distribution function directly at the wall, i.e., the distribution $\bar{f}$ of (4.1), must be equal to the flux computed with the distribution function f_G of the gas just in front of the wall (Struchtrup, 2005b), that is, $\int \Psi_A C_k^W n_k \bar{f} \, \mathrm{d}\mathbf{c} = \int \Psi_A C_k^W n_k f_G \, \mathrm{d}\mathbf{c}$ or

$$\|\Psi_A(C_i^W)\| = \int_{C_k^W n_k \geqslant 0} \Psi_A(C_i^W) C_k^W n_k (\chi f_W + (1-\chi)\tilde{f}_G - f_G) \mathrm{d}\mathbf{c} = 0. \tag{4.4}$$

With some substitutions this can be cast in the form

$$\int \Psi_A C_k^W n_k f_G \, \mathrm{d}\mathbf{c} = \frac{\chi}{1-\chi} \int_{C_k^W n_k \geqslant 0} \Psi_A C_k^W n_k [f_W - f_G] \mathrm{d}\mathbf{c} + \int_{C_k^W n_k \geqslant 0} [\Psi_A - \tilde{\Psi}_A] C_k^W n_k \tilde{f}_G \, \mathrm{d}\mathbf{c}, \tag{4.5}$$

where $\tilde{\Psi}_A = \Psi_A(C_k^W - 2C_j^W n_j n_k)$ is evaluated with inverted normal velocity.

Now, we ask for which moments, and thus for which functions Ψ_A, the above conditions must be evaluated. Grad (1949) argues as follows: for a specularly reflecting wall, where $\chi = 0$, (4.5) reduces to

$$\begin{aligned} &\int \Psi_A C_k^W n_k f_G \, \mathrm{d}\mathbf{c} = 0, && \text{if } \Psi_A \text{ is even in } C_k^W n_k, \\ &\int_{C_k^W n_k \geqslant 0} \Psi_A C_k^W n_k (f_G - \tilde{f}_G) \mathrm{d}\mathbf{c} = 0, && \text{if } \Psi_A \text{ is odd in } C_k^W n_k. \end{aligned} \tag{4.6}$$

Then, in case that the gas distribution is even, $f_G = \tilde{f}_G$, for odd Ψ_A (4.5) reduces to a mere identity, and not to a meaningful boundary condition. Therefore, concludes Grad, boundary conditions for moments must be constructed from (4.5) only for functions Ψ_A that are even in the normal velocity component.

We show boundary conditions constructed such only for 2D geometry, with the wall normal pointing into direction x_2, and x_1 as the tangential direction. Due to the relations (4.3), the conditions $\|\Psi_A(C_k^W)\| = 0$ and $\|\Psi_A(C_k)\| = 0$ are equivalent. Evaluation of (4.5) for $\Psi_A = \{C_1, C^2, C_1^2, C_2^2, C^2 C_1\}$ with the distribution function for the R13 equations gives the boundary conditions (Gu & Emerson, 2007; Torrilhon & Struchtrup, 2008)

$$\sigma_{12} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[P(v_1 - v_1^W) + \frac{1}{5}q_1 + \frac{1}{2}m_{122}\right] n_2$$

$$q_2 = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[2P(\theta - \theta_W) - \frac{1}{2}PV^2 + \frac{1}{2}\theta\sigma_{22} + \frac{1}{15}\Delta + \frac{5}{28}R_{22}\right] n_2$$

$$m_{112} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[\frac{1}{14}R_{11} + \theta\sigma_{11} - \frac{1}{5}\theta\sigma_{22} + \frac{1}{5}P(\theta-\theta_W) - \frac{4}{5}PV^2 + \frac{1}{150}\Delta\right]n_2 \tag{4.7}$$

$$m_{222} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[\frac{2}{5}P(\theta-\theta_W) - \frac{3}{5}PV^2 - \frac{7}{5}\theta\sigma_{22} + \frac{1}{75}\Delta - \frac{1}{14}R_{22}\right]n_2$$

$$R_{12} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[P\theta(v_1 - v_1^W) - \frac{11}{5}q_1 - \frac{1}{2}\theta m_{122} - PV^3 + 6PV(\theta-\theta_W)\right]n_2.$$

Here, v_1^W and θ_W are the velocity and temperature of the wall, and $P = \rho\theta + \frac{1}{2}\sigma_{22} - \frac{1}{120}\frac{\Delta}{\theta} - \frac{1}{28}\frac{R_{22}}{\theta}$. Vanishing normal velocity, $v_2 = 0$, is already incorporated into the above.

The first two equations describe velocity slip and temperature jump at the wall. An equivalent set of boundary conditions for the linearized R13 equations was found from phenomenological thermodynamic arguments in Struchtrup & Torrilhon (2007b). For extended moment systems, e.g., the R26 equations, additional boundary conditions are required which follow from the same set of arguments by using the appropriate extended phase density (Gu & Emerson, 2009; Gu *et al.*, 2010).

4.4 *Slip and jump conditions for NSF*

Classical hydrodynamics—the NSF equations—requires only boundary conditions for velocity and temperature, that is, the first two conditions (4.7) on each side of the domain. Different levels of accuracy can be achieved for these boundary conditions, depending on the gas distribution function that is used for evaluation. If only the first approximation (3.9) is used, one finds the first-order jump and slip boundary conditions

$$\begin{aligned} v_1 - v_1^W &= -\frac{2-\chi}{\chi}\sqrt{\frac{\pi\theta}{2}}\frac{\sigma_{12}^{(1)}}{p} - \frac{1}{5}\frac{q_1^{(1)}}{p}, \\ \theta - \theta_W &= -\frac{2-\chi}{\chi}\sqrt{\frac{\pi\theta}{8}}\frac{q_2^{(1)}}{p} + \frac{1}{4}\theta\frac{\sigma_{22}^{(1)}}{p}. \end{aligned} \tag{4.8}$$

Experience shows that the capability of the NSF equations for the prediction of rarefied flow phenomena can be improved by second-order slip conditions (Deissler, 1964; Lockerby *et al.*, 2004; Hadjiconstantinou, 2006). By making use of geometry and scaling arguments, the R13 equations can be used to construct higher-order boundary conditions from $(4.7)_{1,2}$. As an example, we show the result for plane channel flows, where slip and jump conditions read (Struchtrup & Torrilhon, 2008)

$$\begin{aligned} v_1 - v_1^W &= -\frac{2-\chi}{\chi}\sqrt{\frac{\pi\theta}{2}}\frac{\sigma_{12}^{(1)}}{p}n_2 + \frac{5}{6}\frac{\mu\theta}{p^2}\frac{\partial\sigma_{12}^{(1)}}{\partial x_2} - \frac{19}{18}\frac{\sigma_{12}^{(1)}q_2^{(1)}}{p^2}, \\ \theta - \theta_W &= -\frac{2-\chi}{\chi}\sqrt{\frac{\pi\theta}{8}}\frac{q_2^{(1)}}{p}n_2 + \frac{17}{35}\frac{\mu}{\rho p}\frac{\partial q_2^{(1)}}{\partial x_2} + \left[\frac{\pi}{8}\left(\frac{2-\chi}{\chi}\right)^2 + \frac{71}{1470}\right]\frac{\sigma_{12}^{(1)}\sigma_{12}^{(1)}}{\rho p} - \frac{178}{525}\frac{q_2^{(1)}q_2^{(1)}}{p^2}. \end{aligned} \tag{4.9}$$

Similar equations can be obtained for cylindrical channel flows (Taheri & Struchtrup, 2009, 2010a).

4.5 *Boundary conditions for the Burnett equations*

As said earlier, to our knowledge, a detailed discussion of the number of boundary conditions required for the Burnett or super-Burnett equations is not available in the literature. Thus, it is presently unclear how many and which boundary conditions should be used for their solution. Obviously, second-order jump and slip boundary conditions must be used, but one would expect the need for additional conditions.

For some problems, in particular flow between parallel plates, the Burnett equations decouple somewhat, so that for the computation of the velocity and temperature fields second-order jump and slip conditions suffice (Lockerby & Reese, 2003; Bao & Lin, 2008; Uribe & Garcia, 1999). However, additional conditions are required to find the density and pressure distribution, and these are unclear (Lockerby & Reese, 2003; Bao & Lin, 2008). Uribe & Garcia (1999) fit to DSMC data to show that the Burnett equations can give meaningful results.

A complete theory of boundary conditions for Burnett equations, however, is currently lacking. Therefore, it is not possible to use these equations for analysis of more complicated flows. Most importantly, the time instability of the equations makes it impossible to produce reliable solutions for time-dependent problems or from time-dependent numerical methods like time stepping into steady state. We recommend to use moment equations instead, in particular regularized equations, which are stable, and are furnished with a complete theory of boundary conditions.

5. Bulk effects and Knudsen layers

In the introduction, we listed the most important rarefaction phenomena. Space limitation prevents us from showing that the R13 equations can indeed accurately describe all of these, provided that the associated Knudsen number does not exceed $\mathrm{Kn} \simeq 0.5$.

The early publications on the R13 equations focused on boundary-free problems, in particular their linear stability, their agreement with measured phase speeds and attenuation of ultrasound waves (Struchtrup & Torrilhon, 2003; Struchtrup, 2004b), and their ability to predict smooth shock structures (Torrilhon & Struchtrup, 2004; Torrilhon, 2006) solved a 2D shock–bubble interaction. The evaluation of the linearized equation already gave evidence that, other than the Burnett-type equations, the R13 equations exhibit Knudsen boundary layers (Struchtrup & Torrilhon, 2003; Struchtrup, 2005a; Struchtrup & Thatcher, 2007a), however, agreement to DSMC simulations was reached by fitting of integration constants, not by applying a complete set of boundary conditions.

The path to fitting-free solutions of boundary-value problems was opened when Gu and Emerson applied Grad's ideas on boundary conditions to the R13 equations (Gu & Emerson, 2007). Their numerical solutions showed spurious sub-Knudsen layers at the walls, which are an artefact of their numerical method, which prescribes more boundary conditions as are mathematically required. After this issue was clarified in Torrilhon & Struchtrup (2008), the door was open to solve the R13 equations for Couette and Poiseuille flow in flat (Taheri *et al.*, 2009b) and cylindrical (Taheri & Struchtrup, 2009, 2010a) geometries, for linear and non-linear transpiration flow (Taheri & Struchtrup, 2010b), and some linear time-dependent problems (Taheri *et al.*, 2009a). Corresponding results for the R26 equations in for flat geometry are presented in Gu & Emerson (2009); Gu *et al.* (2009) and Gu *et al.* (2010).

5.1 *Poiseuille flow*

A particularly important feature of the R13 and R26 equations is that they are accessible to analytical solutions of boundary-value problems, even for somewhat non-linear processes. As an example, we

study the analytical results for force-driven Poiseuille flow between infinite resting parallel plates of uniform temperature θ_W (Taheri *et al.*, 2009b). This flow is dominated by shear, and thus quadratic terms in shear-related quantities such as shear stress and velocity gradients were kept in the R13 equations, while they were linearized else. The analytical results for the relevant variables read

$$
\begin{aligned}
v_1 &= \underline{\mathsf{C}_1 G_1 - \frac{G_1 x_2^2}{2\mathrm{Kn}}} - \frac{2}{5} q_1, \\
\theta &= \underline{\theta_W + \mathsf{C}_2 G_1^2 - \frac{1}{45}\frac{G_1^2 x_2^4}{\mathrm{Kn}^2}} + \frac{488}{525} G_1^2 x_2^2 + \mathsf{C}_3 G_1 \left[\frac{956}{375} G_1 \mathrm{Kn} \cosh \frac{\sqrt{5} x_2}{3\mathrm{Kn}} + \frac{32\sigma_{12}}{35\sqrt{5}} \sinh \frac{\sqrt{5} x_2}{3\mathrm{Kn}} \right] \\
&\quad - \mathsf{C}_4 G_1^2 \frac{2}{5} \cosh \frac{\sqrt{5} x_2}{\sqrt{6}\mathrm{Kn}}, \\
\sigma_{12} &= \underline{G_1 x_2}, \\
\sigma_{22} &= -\frac{84 G_1^2 \mathrm{Kn}^2}{25} - \frac{6}{5} G_1^2 x_2^2 - \mathsf{C}_3 G_1 \left[\frac{152}{25} G_1 \mathrm{Kn} \cosh \frac{\sqrt{5} x_2}{3\mathrm{Kn}} + \frac{12\sigma_{12}}{5\sqrt{5}} \sinh \frac{\sqrt{5} x_2}{3\mathrm{Kn}} \right] \\
&\quad + \mathsf{C}_4 G_1^2 \cosh \frac{\sqrt{5} x_2}{\sqrt{6}\mathrm{Kn}}, \\
q_1 &= -\frac{3}{2} G_1 \mathrm{Kn} + \mathsf{C}_3 G_1 \cosh \frac{\sqrt{5} x_2}{3\mathrm{Kn}}, \\
q_2 &= \underline{\frac{1}{3}\frac{G_1^2 x_2^3}{\mathrm{Kn}}} - \mathsf{C}_3 G_1 \left[\frac{6}{5\sqrt{5}} G_1 \mathrm{Kn} \sinh \frac{\sqrt{5} x_2}{3\mathrm{Kn}} - \frac{2}{5} \sigma_{12} \cosh \frac{\sqrt{5} x_2}{3\mathrm{Kn}} \right].
\end{aligned}
\tag{5.1}
$$

and the R13 constitutive equations (3.16) reduce to

$$
\begin{aligned}
\Delta &= -2\sigma_{12}^2 - 12\mathrm{Kn}\left(\frac{\mathrm{d}q_2}{\mathrm{d}x_2} + \sigma_{12} \frac{\mathrm{d}v_1}{\mathrm{d}x_2} \right), \\
R_{12} &= -\frac{12}{5}\mathrm{Kn}\frac{\mathrm{d}q_1}{\mathrm{d}x_2}, \\
R_{22} &= -\frac{4}{21}\sigma_{12}^2 - \frac{16}{5}\mathrm{Kn}\left(\frac{\mathrm{d}q_2}{\mathrm{d}x_2} + \frac{5}{14}\sigma_{12}\frac{\mathrm{d}v_1}{\mathrm{d}x_2} \right), \\
m_{122} &= -\frac{16}{15}\mathrm{Kn}\frac{\mathrm{d}\sigma_{12}}{\mathrm{d}x_2}, \\
m_{222} &= -\frac{6}{5}\mathrm{Kn}\left(\frac{\mathrm{d}\sigma_{22}}{\mathrm{d}x_2} - \frac{4}{15} q_1 \frac{\mathrm{d}v_1}{\mathrm{d}x_2} \right).
\end{aligned}
$$

Here, all quantities are made dimensionless, G_1 is the (dimensionless) force that drives the flow and C_α are the integrating constants that must be determined from the boundary conditions (4.5). We have made

their dependence on G_1 explicit, so that the C_α are numbers that depend on Knudsen number; to save space, their details are not shown.

In the above solution, those terms that would be present in the classical description of the process via the NSF equations are underlined. Thus, all terms that are not underlined describe rarefaction phenomena.

Before we discuss these, we have a short look at the NSF solution, which reads

$$v_1^{(\mathrm{NSF})} = \mathsf{C}_1 G_1 - \frac{G_1 x_2^2}{2\mathrm{Kn}}, \quad \sigma_{12}^{(\mathrm{NSF})} = G_1 x_2, \quad \sigma_{22}^{(\mathrm{NSF})} = 0$$

$$\theta^{(\mathrm{NSF})} = \theta_W + \mathsf{C}_2 G_1^2 - \frac{1}{45}\frac{G_1^2 x_2^4}{\mathrm{Kn}^2}, \quad q_2^{(\mathrm{NSF})} = \frac{1}{3}\frac{G_1^2 x_2^3}{\mathrm{Kn}}, \quad q_1^{(\mathrm{NSF})} = 0.$$

The result is well known: the velocity profile is parabolic, while shear stress is linear. Viscous dissipation in the energy balance leads to a fourth-order temperature profile, and a corresponding heat flux q_2 towards the walls. There are no normal stresses (σ_{22}) and there is no heat flux q_1 into the direction of the flow. Temperature profile and heat flux q_2 are non-linear effects as can be seen by the occurrence of the square of G_1.

With the NSF results in mind, we return to the solution (5.1) of the R13 equations. The—ununderlined—rarefaction terms can be split into two groups: Knudsen layer effects and bulk effects.

All contributions with hyperbolic sine and cosine functions describe Knudsen layers. These terms describe exponential decay away from the wall over few mean free paths. For small Knudsen numbers, the Knudsen layers are limited to the vicinity of the wall, but for larger Knudsen numbers, they contribute to the flow anywhere in the domain. In fact, linear rarefied flows can be dominated by Knudsen layers.

The other contributions are bulk effects, most of which are non-linear in the driving force G_1. For small Knudsen numbers, these terms can be ignored against the—underlined—hydrodynamic contributions, but for finite-Knudsen numbers they contribute considerably.

A particularly interesting effect can be seen in the equation for temperature θ which contains the two terms $\frac{G_1^2}{45\mathrm{Kn}^2}\left[-x_2^4 + \frac{1465}{35}\mathrm{Kn}^2 x_2^2\right]$. The first term is the hydrodynamic contribution, and the second term is a non-linear bulk rarefaction effect. Since both terms have different sign, they compete, which leads to a significant dip in the temperature curve. This dip can be found from analytical considerations of the Boltzmann equation and from its numerical solution (Alaoui & Santos, 1992; Tij & Santos, 1994; Tij *et al.*, 1998; Mansour *et al.*, 1997; Aoki *et al.*, 2002; Zheng *et al.*, 2002; Xu, 2003; Xu & Li, 2004). This phenomenon can only be captured by a macroscopic model that is accurate to super-Burnett order.

Although there is no temperature gradient in flow direction, there is a heat flux q_1 in flow direction, which is also well established in kinetic theory (Baranyai *et al.*, 1992; Todd & Evans, 1995, 1997; Uribe & Garcia, 1999; Aoki *et al.*, 2002).

Figure 1, reprinted from Taheri *et al.* (2009b), shows plots for the relevant moments for a variety of Knudsen numbers. The comparison to DSMC simulations shows good agreement. We point out that the temperature θ and heat flux q_2 are governed by non-linear bulk effects, while the heat flux q_1 is governed by Knudsen layers only, and the normal stress σ_{22} curve results from the interplay of Knudsen layers and bulk effects. Thus, the figure gives good evidence that the R13 equations can describe both classes of rarefaction phenomena: Knudsen layer effects and (non-linear) bulk effects.

Knudsen layer dominant flow is also encountered in thermal transpiration flow (Sharipov & Seleznev, 1998; Taheri & Struchtrup, 2010b).

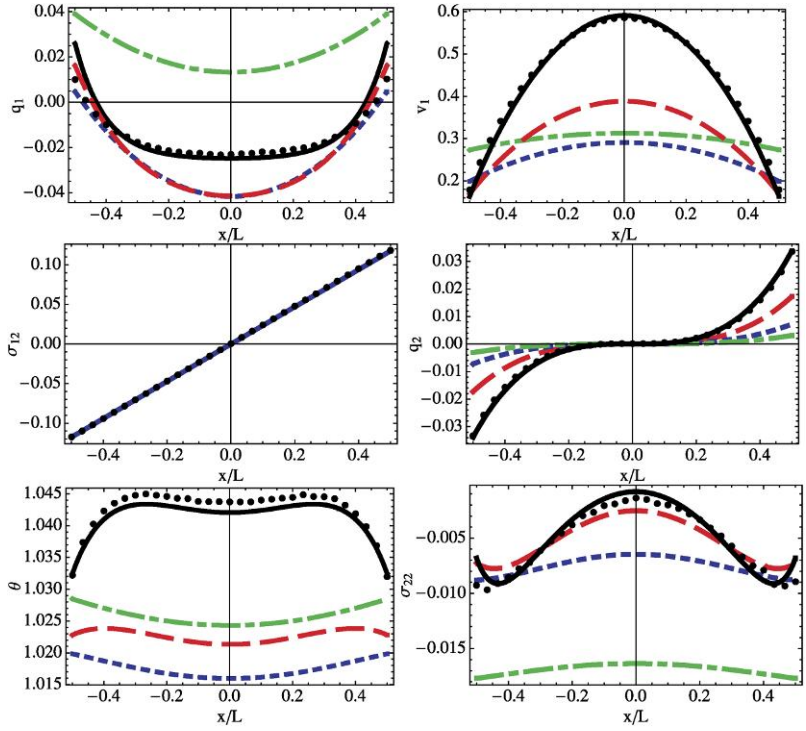

FIG. 1. Force-driven Poiseuille flow with dimensionless force $G_1 = 0.2355$. Profiles are computed for Kn $= 0.072$ (solid line), 0.15 (dashed line), 0.4 (dotted line) and 1.0 (dash-dot line). Circles are DSMC simulations for Kn $= 0.072$ (Taheri *et al.*, 2009b).

5.2 *More on Knudsen layers*

The analytical results for Poiseuille flow (5.1) show that most significant bulk rarefaction effects are non-linear in the driving force. Knudsen layers, on the other hand, are linear effects which will be dominant for linear flow regimes.

As the solution shows, for plane walls, Knudsen layers describe exponential decay away from the boundary of the form $\exp\left[-\gamma \frac{|x|}{\mathrm{Kn}}\right]$ with a numerical coefficient γ of order unity. We recall that $\mathrm{Kn} = \lambda/L$, where λ is the mean free path, and L the length scale of interest which is used to non-dimensionalize the space variable. Thus, the layer extends few mean free paths from the wall into the flow domain. For flows with small Knudsen numbers, the layer is restricted to the close vicinity of the wall, while for flows with larger Knudsen numbers, the layer can extend all through the flow domain. Obviously, when one is interested in resolving the Knudsen layer (KL), the length scale of interest is the mean free path, $L_{\mathrm{KL}} = \lambda$, and the corresponding Knudsen number is unity, $\mathrm{Kn}_{\mathrm{KL}} = 1$.

The CE method relies on an expansion in the Knudsen number, for which the Knudsen number must be well-below unity. It follows that in the CE method Knudsen layers (for which $\mathrm{Kn}_{\mathrm{KL}} = 1$) are not accessible. Accordingly, it is not surprising that the higher CE expansions, i.e., the Burnett and super-Burnett equations do not give the full array of Knudsen layers contributions or even show unphysical oscillations (Struchtrup, 2005a,b).

The full array of moment equations, on the other hand, gives proper Knudsen layers. Moment equations and their Knudsen layers are discussed for a simple kinetic equation in Struchtrup (2008). There it is shown that in the moment framework the actual Knudsen layer is a linear combination of many exponential terms,

$$\mathrm{KL} = \sum A_\alpha \exp\left[-\gamma_\alpha \frac{|x|}{\mathrm{Kn}}\right]. \tag{5.2}$$

The γ_a are numerical coefficients of order unity which give the width of the various contributions, and the A_α are the corresponding amplitudes which are determined from the boundary conditions. The analysis shows that for small Knudsen numbers the amplitudes vanish, so that in this limit—classical hydrodynamics—Knudsen layers can be neglected. For larger Knudsen numbers, the results converge with increasing moment number; converged results require a relatively large number of moments. For smaller number of moments, the Knudsen layer curvature differs from the converged result, but, interestingly, the overall results are surprisingly good. Indeed, the lack of curvature close to the wall is compensated by additional jump at the boundary, so that overall even a small set of moment equations can do well—the moment system with proper boundary conditions finds a best approximation to the boundary-value problem.

The order of magnitude method uses the CE scaling for model reduction, but it does not expand in the Knudsen number. Since the reduction is based on the CE scaling, in fact it aims at getting proper equations for the bulk. However, compared to the CE method, the order of magnitude method is less restrictive. In particular, the method leaves the structure of the moment equations intact, and thus gives Knudsen layers. In other words: while the order of magnitude method does not aim for Knudsen layers, it does not remove them from the moment equations where they are present. The CE expansion also aims at the bulk but removes the Knudsen layers.

We also mention attempts to add modelling of Knudsen layers to the NSF equations by Reese *et al.* (2007) and Lockerby & Reese (2008). In these models, the Knudsen layers are modelled through modifying the Navier–Stokes strain–stress relation close to the wall, with functions and coefficients adjusted to give a best fit with solutions of the Boltzmann equation. Since the models are constructed, but not derived from the Boltzmann equation, it is unclear how good they will be for predicting results for other processes. For instance, the analysis of regularized moment equations shows that in cylindrical problems, the Knudsen layers are Bessel functions (Taheri & Struchtrup, 2009, 2010a) and not exponentials as in flat geometry. Thus, result for flat geometry cannot be just extrapolated to curved geometry. Moreover, these models do not incorporate Knudsen layers and bulk rarefaction effects for higher moments such as heat flux and stress, and thus are not able to predict important features of rarefied gas flows. In our opinion, a closed set of equations—here, the R13 or R26 equations—that is derived from the underlying microscopic behaviour—here, the Boltzmann equation—is preferable over fitted equations with unclear range of applicability.

5.3 *R13 and R26 equations and beyond*

The R13 equations are the smallest set of moment equations that describes Knudsen layer effects for the 13 variables $\{\rho, v_i, \theta, \sigma_{ij}, q_i\}$, moreover, they are accurate to super-Burnett order in the bulk. They give accurate results for Knudsen numbers up to $\mathrm{Kn} \simeq 0.5$. Extending the number of moments adds more Knudsen layer contributions, see (5.2), and thus gives more accurate description of these, while it also increases the accuracy in the bulk to orders above super-Burnett.

The R26 moment equations allow a more accurate description of Knudsen layers (Gu & Emerson, 2009; Gu *et al.*, 2009; Gu *et al.*, 2010), their bulk accuracy should be of fifth order (Struchtrup, 2005b). Numerical solutions of the R26 equations show that they extend the range towards larger Knudsen numbers of up to Kn $\simeq$ 1.0.

For microflow problems Knudsen layer effects dominate, while higher-order bulk effects are less important. For these problems, somewhat linearized versions of the equations are highly useful, as demonstrated for the R13 equations by Taheri *et al.* (2009b). To reduce the numerical effort, a similar reduction could be done for the R26 equations, so that high-order non-linearities are removed.

Increasing the moment number further, say to 45 or moments (Struchtrup, 2005b), will yield better results, but this comes at the price of having to handle an even larger array of equations and boundary conditions. The aim of a moment system must be to obtain good results at reduced effort, which becomes more difficult for larger systems. The preparation of the equations for numerical codes becomes more complex for more extended systems, the more so when one makes use of the geometry—already the formulation of the R13 equations in cylindrical geometry was quite cumbersome (Taheri & Struchtrup, 2009, 2010a).

6. Conclusions and outlook

Macroscopic transport equations can be reliable tools for the description of rarefied gas flows for not too large Knudsen numbers. A successful model must be able to describe bulk rarefaction effects and Knudsen layers, as well as their interplay.

Due to their derivation from an expansion in the Knudsen number, models obtained from the CE expansion, i.e., the Burnett and super-Burnett equations, fail to give Knudsen layers for all variables. Moreover, these equations suffer from instabilities in time-dependent problems and are not accompanied by a full set of boundary conditions. While the equations can describe some of the rarefaction phenomena in the bulk, they have so many disadvantages that they cannot be considered as a reliable tool for the description of rarefied gas flows.

Reduced moment systems, like the R13 and R26 equations, describe Knudsen layers and bulk rarefaction effects well. The R13 equations predict flows with Kn $<$ 0.5 with errors below $\sim$5–7%. For larger Knudsen numbers, the equations still describe the qualitative behavior well, and thus will be useful for the understanding of rarefied flow phenomena. The R26 equations allow to extend the range of accuracy to Kn$<$1 with errors below $\sim$5–7%.

These equations are stable and are furnished with complete boundary conditions, and thus are accessible for a wide array of problems—as long as the Knudsen number of the process does not exceed the limit of validity for the respective set of equations. At present, the R13 and R26 moment equations, with their boundary conditions, are the only macroscopic models that can describe Knudsen layers and bulk effects with sufficient accuracy.

Macroscopic models for rarefied flows have two particularly appealing features. (a) The equations can be solved analytically for linear and non-linear problems. The analytical solutions offer additional insight into rarefaction phenomena, and on the influence the various macroscopic quantities have on each other. (b) The equations are accessible to numerical solutions with various methods. Most solvers for the Boltzmann equation use time stepping into steady state for finding steady-state solutions, which is costly due to the stiffness of the equation. Due to the reduced number of variables, time stepping is considerably cheaper for moment systems (Gu & Emerson, 2007; Gu & Emerson, 2009), but it can be avoided altogether with suitable codes (Torrilhon & Struchtrup, 2008). We are presently extending the numerical method of Torrilhon & Struchtrup (2008) for 2D flow; preliminary results indicate

computational times of minutes for processes that need days for the solution of the Boltzmann equation, while showing good agreement to the latter.

Together with suitable numerical methods, the regularized moment equations with 13 or 26 moments offer a reliable tool for the description of rarefied gas flows with Knudsen numbers below unity. The equations capture all thermal and kinematic rarefaction phenomena—linear and non-linear—at a fraction of the numerical cost of microscopic solvers.

So what needs to be done in the future? (a) Fast numerical methods for complex geometries are mandatory. (b) Solutions of open systems, e.g., a micro-pipe connecting two pressurized and thermalized containers, require inflow and outflow conditions to avoid computation of the containers—up to now this problem was not tackled. (c) Currently, regularized moment equations are available only for monatomic gases. Since most gases of technical interest are diatomic (air!), or polyatomic, the theory must be extended to go beyond the monatomic gas. (d) Similarly, many technical applications deal with gas mixtures (air, again!)—a macroscopic theory for mixtures is desirable. (e) A deeper understanding of the mathematical structure of the extended equations could contribute to the development of better numerical methods. (f) Presently, the H-theorem (second law of thermodynamics) is available only for the linearized equations, the extension to the non-linear equations would be desireable.

Funding

Natural Sciences and Engineering Research Council (NSERC) (239199-06).

References

ALAOUI, M. & SANTOS, A. (1992) Poiseuille flow driven by an external force. *Phys. Fluids A*, **4**, 1273–1282.

ALSMEYER, H. (1976) Density profiles in argon and nitrogen shock waves measured by the absorbtion of an electron beam. *J. Fluid Mech.*, **74**, 497.

ANSUMALI, S., KARLIN, I. V., ARCIDIACONO, S., ABBAS, A. & PRASIANAKIS, N. I. (2007) Hydrodynamics beyond Navier-Stokes: exact solutions to the lattice Boltzmann hierarchy. *Phys. Rev. Lett.*, **98**, 124502.

AOKI, K., TAKATA, S. & NAKANISHI, T. (2002) Poiseuille type flow of a rarefied gas between two parallel plates driven by a uniform external force. *Phys. Rev. E*, **65**, 026315.

AU, J. D., TORRILHON, M. & WEISS, W. (2001) The shock tube study in extended thermodynamics. *Phys. Fluids*, **13**, 2423–2432.

BAO, F. & LIN, J. (2008) Burnett simulation of gas flow and heat transfer in micro Poiseuille flow. *Int. J. Heat Mass Transf.*, **51**, 4139–4144.

BARANYAI, A., EVANS, D. J. & DAIVIS, P. J. (1992) Isothermal shear-induced heat-flow. *Phys. Rev. A*, **46**, 7593–7600.

BHATNAGAR, P. L., GROSS, E. P. & KROOK, M. (1954) A Model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems. *Phys. Rev.*, **94**, 511–525.

BIRD, G. (1994) *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford: Clarendon Press.

BOBYLEV, A. V. (1982) The Chapman-Enskog and grad methods for solving the Boltzmann equation. *Sov. Phys. Dokl.*, **27**, 29–31.

BOBYLEV, A. V. (2006) Instabilities in the Chapman-Enskog expansion and hyperbolic Burnett equations. *J. Stat. Phys.*, **124**, 371–399.

BURNETT, D. (1936) The distribution of molecular velocities and the mean motion in a non-uniform gas. *Proc. Lond. Math. Soc.*, **40**, 382–435.

CERCIGNANI, C. (1975) *Theory and Application of the Boltzmann Equation*. Edinburgh: Scottish Academic Press.

CHAPMAN, S. & COWLING, T. G. (1970) *The Mathematical Theory of Non-Uniform Gases*. Cambridge: Cambridge University Press.

DEISSLER, R. G. (1964) An analysis of second order slip flow and temperature jump boundary conditions for rarefied gases. *Int. J. Heat Mass Transf.*, **7**, 681–694.

DREYER, W. (1987) Maximization of the entropy in non-equilibrium. *J. Phys. A Math. Gen.*, **20**, 6505.

DREYER, W., JUNK, M. & KUNIK, M. (2001) On the approximation of the Fokker-Planck equation by moment systems. *Nonlinearity*, **14**, 881–906.

FERZIGER, J. H. & KAPER, H. G. (1972) *Mathematical Theory of Transport Processes in Gases*. Amsterdam, The Netherlands: North-Holland.

FISCKO, K. A. & CHAPMAN, D. R. (1989) Comparison of Burnett, super-Burnett and Monte Carlo solutions for hypersonic shock structure. *Proceedings of the 16th Symposium on Rarefied Gasdynamics* (E. P. Muntz, D. Weaver & D. Campbell eds). Washington, DC: AIAA, pp. 374–395.

GARCÍA-COLÍN, L. S., VELASCO, R. M. & URIBE, F. J. (2008) Beyond the Navier–Stokes equations: Burnett hydrodynamics. *Phys. Rep.*, **465**, 149–189.

GILBARG, D. & PAOLUCCI, D. (1953) The structure of shock waves in the continuum theory of fluids. *J. Rat. Mech. Anal.*, **2**, 617–642.

GRAD, H. (1949) On the kinetic theory of rarefied gases. *Commun. Pure Appl. Math.*, **2**, 331–407.

GRAD, H. (1958) Principles of the kinetic theory of gases. *Handbuch der Physik XII: Thermodynamik der Gase* (S. Flügge ed.). Berlin: Springer, pp. 205–294.

GREENSPAN, M. (1956) Propagation of sound in five monatomic gases. *J. Acoust. Soc. Am.*, **28**, 644–648.

GU, X. J. & EMERSON, D. (2007) A computational strategy for the regularized 13 moment equations with enhanced wall-boundary conditions. *J. Comput. Phys.*, **225**, 263–283.

GU, X. J. & EMERSON, D. R. (2009) A high-order moment approach for capturing non-equilibrium phenomena in the transition regime. *J. Fluid Mech.*, **636,** 177–216.

GU, X. J. EMERSON, D. R. & TANG, G. T. (2009) Kramers' problem and the Knudsen minimum: a theoretical analysis using a linearized 26-moment approach. *Cont. Mech. Thermodyn.*, **21**, 345–360.

GU, X. J. EMERSON, D. R. & TANG, G. H. (2010) Analysis of the slip coefficient and defect velocity in the Knudsen layer of a rarefied gas using the linearized moment equations. *Phys. Rev. E*, **81**, 016313.

HADJICONSTANTINOU, N. G. (2006) Comment on Cercignani's second-order slip coefficient. *Phys. Fluids*, **15**, 2352–2354.

HICKEY, K. A. & LOYALKA, S. K. (1990) Plane Poiseuille flow: rigid sphere gas. *J. Vac. Sci. Technol. A*, **8**, 735–1259.

HOLIAN, B. L., PATTERSON, C. W., MARESCHAL, M. & SALOMONS, E. (1993) Modeling shock waves in an ideal gas: going beyond the Navier-Stokes level. *Phys. Rev. E*, **47**, R24–R27.

JIN, S., PARESCHI, L. & SLEMROD, M. (2002) A relaxation scheme for solving the Boltzmann equation based on the Chapman-Enskog expansion. *Acta Math. Appl. Sin. Engl. Ser*., **18**, 37–62.

JIN, S. & SLEMROD, M. (2001) Regularization of the Burnett equations via relaxation. *J. Stat. Phys.*, **103**, 1009–1033.

JUNK, M. (1998) Domain of definition of Levermore's five-moment system. *J. Stat. Phys.*, **93**, 1143–1167.

JUNK, M. (2003) Maximum entropy moment problems and extended Euler equations. *Transport in Transition Regimes* (N. B. Abdallah, A. Arnold, P. Degond, I. Gamba, R. Glassey, C. D. Levermore & C. Ringhofer eds). IMA Vol. Math. Appl., vol. 135. New York: Springer, pp. 189–198.

KARLIN, I. V., GORBAN, A. N., DUKEK, G. & NONNENMACHER, T. F. (1998) Dynamic correction to moment approximations. *Phys. Rev. E*, **57**, 1668–1672.

KNUDSEN, M. (1909) Die Gesetze der Molekularströmung und der inneren Reibungsströmung der Gase durch Röhren. *Ann. Phys.*, **333**, 75–130.

KOGAN, M. N. (1969) *Rarefied Gas Dynamics*. New York: Plenum Press.

LEVERMORE, C. D. (1996) Moment closure hierarchies for kinetic theories. *J. Stat. Phys.*, **83**, 1021–1065.

LOCKERBY, D. A. & REESE, J. M. (2003) High resolution Burnett simulation of micro Couette flow and heat transfer. *J. Comput. Phys.* **188**, 333–347.

LOCKERBY, D. A. & REESE, J. M. (2008) On the modelling of isothermal gas flows at the microscale. *J. Fluid Mech.,* **604**, 235–261.

LOCKERBY, D. A., REESE, J. M., EMERSON, D. R. & BARBER, R. W. (2004) Velocity boundary condition at solid walls in rarefied gas calculations. *Phys. Rev. E,* **70**, 017303.

MANSOUR, M. M., BARAS, F. & GARCIA, A. L. (1997) On the validity of hydrodynamics in plane Poiseuille flows. *Physica A,* **240**, 255–267.

MARQUES JR, W. & KREMER, G. M. (2001) Couette flow from a thirteen field theory with jump and slip boundary conditions. *Cont. Mech. Thermodyn.*, **13**, 207–217.

MÜLLER, I. M, REITEBUCH, D. & WEISS, W. (2003) Extended thermodynamics—consistent in order of magnitude. *Cont. Mech. Thermodyn*, **15**, 113–146.

MÜLLER, I. M & RUGGERI, T. (1998) *Rational Extended Thermodynamics*. New York: Springer. (Springer Tracts in Natural Philosophy, Vol. 37.)

OHWADA, T., SONE, Y. & AOKI, K. (1989) Numerical analysis of the Poiseuille and thermal transpiration flows between two parallel plates on the basis of the Boltzmann equation for hard-sphere molecules. *Phys. Fluids A,* **1**, 2042–2049.

ÖTTINGER, H. C. (2010a) Thermodynamically admissible 13 moment equations from the Boltzmann equation. *Phys. Rev. Lett.*, **104**, 120601.

ÖTTINGER, H. C. (2010b) Öttinger replies. *Phys. Rev. Lett.*, **105**, 128902.

REESE, J. M., ZHENG, Y. & LOCKERBY, D. A. (2007) Computing the near-wall region in gas micro- and nanofluidics: critical Knudsen layer phenomena. *J. Comput. Theor. Nanosci.*, **4**, 807–813.

REINECKE, S. & KREMER, G. M. (1990) Method of moments of grad. *Phys. Rev. A*, **42**, 815–820.

REINECKE, S. & KREMER, G. M. (1996) Burnett's equations from a (13+9N)-field theory. *Cont Mech. Thermodyn.*, **8**, 121–130.

REITEBUCH, D. & WEISS, W. (1999) Application of high moment theory to the plane couette flow. *Cont. Mech. Thermodyn.*, **11**, 217–225.

RISSO, D. & CORDERO, P. (1998) Generalized hydrodynamics for a Poiseuille flow: theory and simulations, *Phys. Rev. E*, **58**, 546–553.

ROSENAU, P. (1989) Extending hydrodynamics via the regularization of the Chapman-Enskog solution, *Phys. Rev. A.*, **40**, 7193–7196.

SHARIPOV, F. & SELEZNEV, V. (1998) Data on internal rarefied gas flows, *J. Phys. Chem. Ref. Data*, **27**, 657–706.

SHAVALIYEV, M. SH. (1993) Super-Burnett corrections to the stress tensor and the heat flux in a gas of Maxwellian molecules. *J. Appl. Math. Mech.*, **57**, 573–576.

SÖDERHOLM, L. H. S (2007) Hybrid Burnett equations: a new method of stabilizing, *Trans. Theory Stat. Phys.*, **36**, 495–512.

SONE, Y. (2002) Kinetic Theory and Fluid Dynamics. Boston, MA: Birkhäuser.

STRUCHTRUP, H. (2002) Heat transfer in the transition regime: solution of boundary value problems or Grad's moment equations via kinetic schemes. *Phys. Rev. E.*, **65**, 041204.

STRUCHTRUP, H. (2003a) Grad's moment equations for microscale flows Symposium on Rarefied Gasdynamics 23. AIP Conf. Proc., **663**, 792–799.

STRUCHTRUP, H. (2003b) Some remarks on the equations of Burnett and Grad. *Transport in Transition Regimes* (N. B. Abdallah, A. Arnold, P. Degond, I. Gamba, R. Glassey, C. D. Levermore & C. Ringhofer eds). IMA Volume, vol. 135. New York: Springer, pp. 265–278.

STRUCHTRUP, H. (2004a) Derivation of 13 moment equations for rarefied gas flow to second order accuracy for arbitrary interaction potentials. *SIAM Multiscale Model. Sim.*, **3**, 211–243.

STRUCHTRUP, H. (2004b) Stable transport equations for rarefied gases at high orders in the Knudsen number. *Phys. Fluids*, **16**, 3921–3934.

STRUCHTRUP, H. (2005a) Failures of the Burnett and super-Burnett equations in steady state processes. *Cont. Mech. Thermodyn.*, **17**, 43–50.

STRUCHTRUP, H. (2005b) *Macroscopic Transport Equations for Rarefied Gas Flows—Approximation Methods in Kinetic Theory*. Interaction of Mechanics and Mathematics Series. Heidelberg: Springer.

STRUCHTRUP, H. (2008) Linear kinetic heat transfer: moment equations, boundary conditions, and Knudsen layers. *Physica A*, **387**, 1750–1766.

STRUCHTRUP, H. & THATCHER, T. (2007a) Bulk equations and Knudsen layers for the regularized 13 moment equations. *Cont. Mech. Thermodyn.*, **19**, 177–189.

STRUCHTRUP, H. & TORRILHON, M. (2003) Regularization of Grad's 13-moment-equations: derivation and linear analysis, *Phys. Fluids*, **15**, 2668–2680.

STRUCHTRUP, H. & TORRILHON, M. (2007b) H-theorem, regularization, and boundary conditions for linearized 13 moment equations, *Phys. Rev. Lett.*, **99**, 014502.

STRUCHTRUP, H. & TORRILHON, M. (2008) Higher-order effects in rarefied channel flows. *Phys. Rev. E*, **78**, 046301, Erratum: *Phys. Rev. E*, **78**, 069903.

STRUCHTRUP, H. & TORRILHON, M. (2010) Comment on Thermodynamically admissible 13 moment equations from the Boltzmann equation. *Phys. Rev. Lett.*, **105**, 128901.

TAHERI, P., RANA, A. S., TORRILHON, M. & STRUCHTRUP, H. (2009a) Macroscopic description of steady and unsteady rarefaction effects in boundary value problems of gas dynamics. *Cont. Mech. Thermodyn.*, **21**, 423–443.

TAHERI, P. & STRUCHTRUP, H. (2009) Effects of rarefaction in microflows between coaxial cylinders. *Phys. Rev. E*, **80**, 066317.

TAHERI, P. & STRUCHTRUP, H. (2010a) An extended macroscopic transport model for rarefied gas flows in long capillaries with circular cross sections. *Phys. Fluids*, **22**, 112004.

TAHERI, P. & STRUCHTRUP, H. (2010b) Rarefaction effects in thermally–driven microflows. *Physica A*, **389**, 30693080.

TAHERI, P., TORRILHON, M. & STRUCHTRUP, H. (2009b) Couette and Poiseuille flows in microchannels: analytical solutions for regularized 13-moment equations. *Phys. Fluids*, **21**, 017102.

TIJ, M., SABBANE, M. & SANTOS, A. (1998) Nonlinear Poiseuille flow in a gas. *Phys. Fluids*, **10**, 1021–1927.

TIJ, M. & SANTOS, A. (1994) Perturbation analysis of a stationary nonequilibrium-flow generated by an external force. *J. Stat. Phys.*, **76**, 1399–1414.

TODD, B. D. & EVANS, D. J. (1995) The heat-flux vector for highly inhomogeneous nonequilibrium fluids in very narrow pores. *J. Chem. Phys.*, **103,** 9804–9809.

TODD, B. D. & EVANS, D. J. (1997) Temperature profile for Poiseuille flow. *Phys. Rev. E.*, **55**, 2800–2807.

TORRILHON, M. (2006) Two-dimensional bulk micro-flow simulations based on regularized Grad's 13-moment-equations. *SIAM Multiscale Model. Sim.*, **5**, 695–728.

TORRILHON, M. & STRUCHTRUP, H. (2004) Regularized 13-moment-equations: shock structure calculations and comparison to Burnett models. *J. Fluid Mech.*, **513**, 171–198.

TORRILHON, M. & STRUCHTRUP, H. (2008) Boundary conditions for regularized 13-moment-equations for micro-channel-flows. *J. Comput. Phys.*, **227**, 1982–2011.

URIBE, F. J. & GARCIA, A. L. (1999) Burnett description for plane Poiseuille flow. *Phys. Rev. E*, **60**, 4063–4078.

URIBE, F. J., VELASCO, R. M. & GARCÍA-COLÍN, L. S. (2000) Bobylev's instability, *Phys. Rev. E*, **62**, 5835–5838.

WEISS, W. (1990) Zur Hierarchie der Erweiterten Thermodynamik. *Ph.D. Thesis*, Technical University Berlin, Berlin, Germany.

WEISS, W. (1995) Continuous shock structure in extended Thermodynamics. *Phys. Rev. E*, **52**, 5760.

XU, K. (2003) Super-Burnett solutions for Poiseuille flow. *Phys. Fluids*, **15**, 2077–2080.

XU, K. & LI, Z. H. (2004) Microchanel flow in the slip regime: gas kinetic BGK–Burnett solutions. *J. Fluid Mech.*, **513**, 87–110.

ZHENG, Y., GARCIA, A. L. & ALDER, B. J. (2002) Comparison of kinetic theory and hydrodynamics for Poiseuille flow. *J. Stat. Phys.*, **109**, 495.

ZHONG, X., MACCORMACK, R. W. & CHAPMAN, D. R. (1993) Stabilization of the Burnett equations and applications to hypersonic flows. *AIAA J.*, **31**, 1036.