

Regularized 13 Moment Equations for Hard Spheres

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Abstract. The regularized 13 moment equations (R13) of rarefied gas dynamics for a monatomic hard sphere gas in the linear regime are presented. The equations are based on an extended Grad-type moment system, which was systematically reduced by means of the Order of Magnitude Method [Struchtrup, Phys. Fluids 16(11), 3921-3934 (2004)]. The linear Burnett and super-Burnett equations are derived from Chapman-Enskog expansion of the R13 equations. While the Burnett coefficients agree with literature values, this seems to be the first time that super-Burnett coefficients are computed for a hard sphere gas. The equations are considered for stability, and dispersion and damping of sound waves. Boundary conditions are given, and solutions of simple boundary value problems are briefly discussed.

Keywords: Rarefied gas flows, Microflows, Regularized 13-moment equations

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INTRODUCTION

Whether gas flows can be described by the classical equations of hydrodynamics—the Navier-Stokes and Fourier laws—depends on the Knudsen number ε of the flow [1–3], which is defined as the ratio between the mean free path of the gas molecules and the typical length scale. Classical hydrodynamics is applicable only for Knudsen numbers below 0.05 or so. For larger Knudsen numbers non-local transport due to relatively large mean free path requires more detailed equations that are able to picture the non-locality. A fully detailed description of the gas flow at all Knudsen numbers is offered by the Boltzmann equation, which solves for the microscopic distribution function of the gas [1, 2]. For many technical applications, in particular those in the so-called transition regime where, roughly, $0.05 \leq \varepsilon \leq 2$, the solution of the Boltzmann equation is rather costly, and provides far more detail than necessary. For flows with large Knudsen numbers the Boltzmann equation is indispensable, but for flows in the transition regime models of extended hydrodynamics offer an alternative [3, 4].

The present paper deals with an extension of a model that we have developed over the last decade, the regularized 13 moment (R13) equations [5–9]. The R13 equations are closely related to Grad’s classical moment method [10], which provides extended sets of equations for rarefied gases. In Grad’s original method the Knudsen number is not used for model reduction, and therefore it is difficult to know which sets of moments one should consider for a given process. Our derivation of the Grad equations and of the R13 equations in [7, 8] by means of the *Order of Magnitude Method* closed this gap, as it provided a clear relation between Knudsen number and the appropriate moment set to consider. The analysis showed that Grad’s 13 moment equations are appropriate to order $\mathcal{O}(\varepsilon^2)$, while the regularized 13 moment equations are of order $\mathcal{O}(\varepsilon^3)$.

Boundary conditions for moments were already discussed by Grad, but systematic solutions of boundary value problems for (regularized) moment equations were studied only recently, after the theory of boundary conditions was fully understood [9, 11]. In several papers we could show that for flows with moderate Knudsen numbers the R13 equations provide accurate predictions in agreement to solutions of the Boltzmann equation, see, e.g., Refs. [12–15].

Burnett and super-Burnett are obtained from the Boltzmann equation by Chapman-Enskog expansion [1, 16, 17] as the second order (Burnett) and third order (super-Burnett) correction to the equations of hydrodynamics. While the Burnett-type equations can describe rarefaction effects in gas flows, they suffer from instabilities that prohibit their use as a predictive tool [20]. Some authors suggested stabilized variants [21, 22]. At present, there is no complete theory of wall boundary conditions available for any of the Burnett-type equations.

In the present paper we discuss the influence of the molecular interaction potential on the transport equations. So far, the R13 equations were developed only for Maxwell molecules, for which the derivation of moment equations is particularly simple, since the moments of the Boltzmann collision term can be computed without a model for the distribution function [1, 3, 24]. For numerical solutions of the Boltzmann equation, one often considers hard sphere

molecules, since for these the numerics of the collision term are easier to handle. Quite often, again for simpler access, the Boltzmann collision term is replaced by kinetic models such as the BGK model [25], the ES-BGK model that corrects the Prandtl number deficiency of the original BGK model [26], and the Shakov model which essentially is a linearized form of the ES-BGK model [27].

On the hydrodynamic level, the main difference between the various models for the collision term in the Boltzmann equation is in the temperature dependence of the viscosity μ , with $\mu \sim T^{0.5}$ for hard spheres, $\mu \sim T$ for Maxwell molecules, and $\mu \sim T^\omega$ for other models (measured value for argon: $\omega = 0.81$). The Prandtl number—the dimensionless ratio of viscosity and heat conductivity—varies only slightly, with a value of $\text{Pr} = \frac{2}{3}$ for Maxwell molecules, and $\text{Pr} = 0.661$ for hard spheres. It is an easy task to incorporate a different temperature dependence of viscosity and a different Prandtl number into the Boltzmann equation, the kinetic models, or the moment equations. Thus, one can mimic the leading order behavior of a gas quite well.

However, viscosity and heat conductivity are not the only transport parameters relevant for a rarefied gas flow. This is best known from the Burnett equations, for which the transport coefficients for a variety of molecular interaction potentials are known [3, 19]. It must be expected that differences in Burnett coefficients due to different molecular interaction potentials are accompanied by visible differences in the prediction of transport quantities.

In the present paper we give some insight into the influence of the molecular interaction potential on the R13 equations. The interaction potential affects the coefficients in the equations and the boundary conditions. The cumbersome derivation of the linearized R13 equations for non-Maxwellian interaction potentials by means of the order of magnitude method [7, 8, 28] is presented in [23]. Space restrictions allow us to present only the resulting equations. The coefficients in the final equations depend in a complicated manner on the interaction potential, and we give values for the case of hard sphere molecules in comparison to Maxwell molecules.

The linearized Burnett and super-Burnett equations can be obtained by Chapman-Enskog expansion of the R13 equations [5, 6]. The Burnett coefficients for hard spheres coincide with the literature values [1, 19]. To our best knowledge, the super-Burnett coefficients, linear or non-linear, were only known for Maxwell molecules [3, 17]. Thus, this seems to be the first time that super-Burnett coefficients are given for non-Maxwellian molecules.

The R13 equations, the Burnett and super-Burnett equations, and their coefficients for Maxwell molecules and hard spheres are presented in Section 2. Section 3 presents, as an interesting first application of the equations, the dispersion and damping of high frequency sound waves with moment and Burnett-type models, comparing predictions for Maxwell molecules and hard spheres. Section 4 gives a short description on the theory of boundary conditions, and the appropriate wall boundary conditions for the R13 equations, with coefficients for Maxwell molecules and hard spheres. Section 5 shows first results for Couette and Poiseuille flows.

TRANSPORT EQUATIONS UP TO THIRD ORDER IN THE KNUDSEN NUMBER

The linearized equations describe transport in a rarefied gas when deviations from a rest state of given temperature and temperature are small. In dimensionless form, the variables are the deviations of density ρ and temperature θ from the rest state, the velocity vector v_i , the anisotropic stress tensor σ_{ij} and the heat flux vector q_i . The dimensionless pressure is given by the linearized ideal gas law $p = 1 + \rho + \theta$, and the dimensionless specific internal energy of the monatomic gas is $u = \frac{3}{2}(1 + \theta)$. The Knudsen number is defined as $\varepsilon = \frac{\mu_0 \sqrt{\theta_0}}{p_0 L}$, where μ_0 is the rest state viscosity, L is the reference length, p_0 is the reference pressure, and θ_0 is the reference temperature in energy units.

The conservation laws for mass, momentum and energy read

$$\frac{\partial \rho}{\partial t} + \frac{\partial v_k}{\partial x_k} = 0, \quad \frac{\partial v_i}{\partial t} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i, \quad \frac{3}{2} \frac{\partial \theta}{\partial t} + \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} = 0 \quad (1)$$

where G_i is the dimensionless body force (e.g., gravity). The conservation laws must be furnished with equations for stress and heat flux, which depend on the Knudsen number order, and the method of derivation. In zeroth order approximation, when the Knudsen number is effectively zero, we have $\sigma_{ij} = q_i = 0$, with which (1) reduce to the linearized Euler equations.

For non-zero Knudsen numbers, the necessary equations depend on the Knudsen number order. For up to third order in the Knudsen number, the order of magnitude method gives the equations [23]

$$\frac{\partial q_i}{\partial t} + a^{(1,1)} \frac{\partial \sigma_{ik}}{\partial x_k} - a^{(1,2)} \frac{\partial \Delta \sigma_{ik}}{\partial x_k} - a^{(1,3)} \varepsilon \frac{\partial}{\partial x_k} \frac{\partial q_{(i}}{\partial x_{k)}} - a^{(1,4)} \varepsilon \frac{\partial^2 q_k}{\partial x_i \partial x_k} = - \frac{a^{(1,0)}}{\varepsilon} \Delta q_i. \quad (2)$$

$$\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)} \frac{\partial q_{(i}}{\partial x_j)} - a^{(2,2)} \frac{\partial \Delta q_{(i}}{\partial x_{(i}} - a^{(2,3)} \underline{\varepsilon} \frac{\partial}{\partial x_k} \frac{\partial \sigma_{ij}}{\partial x_k)} - a^{(2,4)} \underline{\varepsilon} \frac{\partial^2 \sigma_{ij}}{\partial x_k \partial x_k} = - \frac{a^{(2,0)}}{\varepsilon} \Delta \sigma_{ij}, \quad (3)$$

where we used the abbreviations

$$\Delta \sigma_{ij} = \sigma_{ij} - \sigma_{ij}^{(NSF)} = \sigma_{ij} + 2\varepsilon \frac{\partial v_{(i}}{\partial x_j)}, \quad \Delta q_i = q_i - q_i^{(NSF)} = q_i + \varepsilon \frac{5}{2\text{Pr}} \frac{\partial \theta}{\partial x_i} \quad (4)$$

which are deviations of stress and heat flux from the Navier-Stokes and Fourier values. Indices in angular brackets denote symmetric trace-free tensors.

In the equations we have used underlining to distinguish terms of different order in ε . For first order in the Knudsen number it suffices to consider only the not underlined terms on the r.h.s. of the equations, which are the laws of Navier-Stokes and Fourier. For second order in ε one has to add the single-underlined terms on the l.h.s., with which the equations become the generalization of Grad's 13 moment equations. For third order in ε the double-underlined terms must be considered as well, then the equations are the full R13 equations for non-Maxwellian molecules.

The Knudsen number ε is the dimensionless viscosity. The values of the coefficients $a^{(\alpha,\beta)}$ and the Prandtl number Pr depend on the molecular interaction potential, where the order of magnitude method gives for Maxwell molecules [3, 7] and hard spheres [23] the values in Table I. We note differences between the coefficients for Maxwell molecules and hard spheres of up to 25%.

TABLE I. R13 coefficients for Maxwell molecules and Hard Spheres.

| | Pr | $a^{(1,0)}$ | $a^{(1,1)}$ | $a^{(1,2)}$ | $a^{(1,3)}$ | $a^{(1,4)}$ | $a^{(2,0)}$ | $a^{(2,1)}$ | $a^{(2,2)}$ | $a^{(2,3)}$ | $a^{(2,4)}$ |
|----|---------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| MM | 0.66667 | 0.66667 | 1.0 | 0.0 | 2.4 | 2.0 | 1.0 | 0.8 | 0.0 | 2.0 | 0.0 |
| HS | 0.66085 | 0.65006 | 0.78694 | 0.17693 | 2.09248 | 1.50489 | 0.98632 | 0.63125 | 0.09466 | 2.19368 | 0.11447 |

From the Chapman-Enskog expansion we find the following equations for stress and heat flux:

$$q_i = - \frac{5}{2\text{Pr}} \varepsilon \frac{\partial \theta}{\partial x_i} + \varepsilon^2 \left(\frac{\theta_4^B}{2} \frac{\partial^2 v_i}{\partial x_k \partial x_k} + \frac{2}{3} \left(\frac{\theta_4^B}{4} - \theta_2^B \right) \frac{\partial^2 v_k}{\partial x_k \partial x_i} \right) - \varepsilon^3 \left(\theta_1^{sB} \frac{\partial^3 \rho}{\partial x_i \partial x_k \partial x_k} + \theta_2^{sB} \frac{\partial^3 \theta}{\partial x_k \partial x_k \partial x_i} \right) \quad (5)$$

$$\sigma_{ij} = -2\varepsilon \frac{\partial v_{(i}}{\partial x_j)} - \varepsilon^2 \left(\varpi_2^B \frac{\partial^2 \rho}{\partial x_{(i} \partial x_j)} + (\varpi_2^B - \varpi_3^B) \frac{\partial^2 \theta}{\partial x_{(i} \partial x_j)} \right) + \varepsilon^3 \left(\varpi_1^{sB} \frac{\partial^2}{\partial x_{(i} \partial x_j)} \frac{\partial v_k}{\partial x_k} - \varpi_2^{sB} \frac{\partial^2}{\partial x_k \partial x_k} \frac{\partial v_{(i}}{\partial x_j)} \right) \quad (6)$$

The notation for Burnett coefficients follows the literature convention [1]. We have used underlining to distinguish terms of different orders: The un-underlined terms are, again, the laws of Navier-Stokes and Fourier. The single-underlined terms are the Burnett corrections, and the double-underlined terms are the super-Burnett terms. Also the Burnett coefficients depend on the interaction potential. For Maxwell molecules and hard spheres we find the values in Table 2. There are noticeable differences in the coefficients between the two molecule types.

TABLE 2. Burnett and super-Burnett coefficients for Maxwell molecules and Hard Spheres.

| | Pr | θ_2^B | θ_4^B | ϖ_2^B | ϖ_3^B | θ_1^{sB} | θ_2^{sB} | ϖ_1^{sB} | ϖ_2^{sB} |
|----|---------|--------------|--------------|--------------|--------------|-----------------|-----------------|-----------------|-----------------|
| MM | 0.66667 | 5.625 | 3.0 | 2.0 | 3.0 | 0.625 | 9.8125 | 1.66667 | 1.33333 |
| HS | 0.66085 | 5.81945 | 2.42113 | 2.02774 | 2.42113 | 2.21659 | 5.92903 | 0.48049 | 0.77111 |

DAMPING AND DISPERSION OF SOUND WAVES

Dispersion and damping can be measured [29, 30]. For high frequency waves one observes distinct deviations from the prediction of classical hydrodynamics, i.e., the Navier-Stokes-Fourier equations, due to gas rarefaction. For waves the Knudsen number must be formed as the ratio of mean free path to wave length, and since wave length is inversely proportional to frequency, the Knudsen number for high frequency waves is not sufficiently small for the Navier-Stokes-Fourier theory to be valid.

We shall not go into much detail of the computation, which was outlined, for the case of Maxwell molecules, in, e.g., [3, 5, 15]. We shall compare damping and dispersion for the following sets of equations: a) Navier-Stokes-Fourier

(NSF), b) Grad 13 moment equations (G13), c) regularized 13 moment equations (R13), d) Burnett equations, e) super-Burnett equations.

The linear equations are considered in simple one-dimensional geometry where they can be written in the general form

$$\frac{\partial u_A}{\partial t} + \mathcal{A}_{AB}^{(1)} \frac{\partial u_B}{\partial x} + \mathcal{A}_{AB}^{(2)} \frac{\partial^2 u_B}{\partial x^2} + \mathcal{A}_{AB}^{(3)} \frac{\partial^3 u_B}{\partial x^3} + \mathcal{A}_{AB}^{(4)} \frac{\partial^4 u_B}{\partial x^4} = -\mathcal{A}_{AB}^{(0)} u_B \quad (7)$$

with the variable vector u_A and suitable matrices $\mathcal{A}_{AB}^{(\alpha)}$. For Navier-Stokes-Fourier we have $u_A = \{\rho, v, \theta\}$ and $\mathcal{A}_{AB}^{(0)} = \mathcal{A}_{AB}^{(3)} = \mathcal{A}_{AB}^{(4)} = 0$; for G13 we have $u_A = \{\rho, v, \theta, \sigma, q\}$ and $\mathcal{A}_{AB}^{(2)} = \mathcal{A}_{AB}^{(3)} = \mathcal{A}_{AB}^{(4)} = 0$; for R13 we have $u_A = \{\rho, v, \theta, \sigma, q\}$ and $\mathcal{A}_{AB}^{(3)} = \mathcal{A}_{AB}^{(4)} = 0$; for Burnett we have $u_A = \{\rho, v, \theta\}$ and $\mathcal{A}_{AB}^{(0)} = \mathcal{A}_{AB}^{(4)} = 0$; for super-Burnett we have $u_A = \{\rho, v, \theta\}$ and $\mathcal{A}_{AB}^{(0)} = 0$.

For the solution for a periodically driven boundary we make the harmonic wave ansatz

$$u_A(x, t) = \hat{u}_A \exp[i(\omega t - kx)] , \quad (8)$$

where ω is the real frequency, $k = k_r + ik_i$ is the complex wave number and \hat{u}_A is the complex amplitude. The phase velocity of the wave is $v_{ph} = \frac{\omega}{k_r}$, and the damping is $(-k_i)$. For a wave with positive phase velocity (i.e., $k_r > 0$) one will expect a positive damping (i.e., $k_i < 0$) [3].

Inserting the wave ansatz (8) into the general form of the transport equations and performing all derivatives gives the algebraic equation

$$\left(\delta_{AB} i\omega + \mathcal{A}_{AB}^{(0)} - ik \mathcal{A}_{AB}^{(1)} - k^2 \mathcal{A}_{AB}^{(2)} + ik^3 \mathcal{A}_{AB}^{(3)} + k^4 \mathcal{A}_{AB}^{(4)} \right) \hat{u}_B = 0 , \quad (9)$$

which only has non-trivial solutions \hat{u}_B for the complex amplitudes if the determinant of the matrix $\mathfrak{A}_{AB}(k) = (\delta_{AB} i\omega + \dots)$ vanishes. Due to the polynomial structure of the complex matrix, its determinant is a polynomial of degree ν in k , with $\nu = 4$ for NSF and G13, $\nu = 6$ for R13 and Burnett, and $\nu = 8$ for super-Burnett. Solution of the solvability condition $\det \mathfrak{A} = 0$ gives the ν branches of the dispersion relation

$$k_a(\omega) , \quad a = 1, \dots, \nu . \quad (10)$$

While all modes can be induced in an experiment, in a sufficiently long apparatus only the mode with the weakest damping will be observed [15], hence we show only these. Figure 1 shows the inverse dimensionless wave speed $\sqrt{\frac{5}{3}} \frac{1}{v_{ph}} = \sqrt{\frac{5}{3}} \frac{k_r}{\omega}$ and the reduced damping $\left(-\frac{k_i}{\omega}\right)$ as functions of the inverse frequency $\frac{1}{\omega}$ for Maxwell molecules (dashed lines) and hard sphere molecules (continuous lines), respectively. The dots are measurements by Meyer & Sessler [29]. For Burnett and super-Burnett equations there are discontinuities in phase speed, and (hardly visible) kinks in damping due to a switch in modes with lowest damping.

Burnett and super-Burnett equations have unphysical modes with negative damping, which appears in particular for high frequency waves, or waves with small wavelengths. This is well-known for Maxwell molecules [3, 15, 20], and the same behavior is observed for the hard sphere gas. For the super-Burnett gaps in the curves for phase speeds occur where this happens.

For the discussion, we recall that NSF, Grad 13, Burnett and super-Burnett can all be obtained by reduction of the R13 equations. For both molecule types we observe that NSF deviates from R13 already for relatively small frequencies, while Grad13 agrees up to larger frequencies. Similarly, the super-Burnett equations agree with R13 for up to higher frequencies than the Burnett equations.

The comparison with experimental data is somewhat surprising. The Burnett equations for Maxwell molecules have a remarkably good agreement with the data for up to rather large frequencies. Considering that the Burnett equations can be obtained by Chapman-Enskog expansion of the R13 and Grad 13 equations, it is not expected that they give a much better agreement than these. Moreover, the super-Burnett equations, which are of third order in the Knudsen number ε , should give a better agreement than the Burnett equations which are only of second order, but this is not the case. It must be concluded that the good agreement of the Burnett equations for Maxwell molecules is accidental rather than systematic.

Further comparison shows distinct differences between the predictions for Maxwell molecules and hard sphere gas, for which all higher order equations predict lower damping. The differences are of the order of 20% or so, simply a reflection of the difference in transport coefficients, which show similar variation.

The experiments are performed with argon, which is neither a Maxwell gas, nor a hard sphere gas, but probably is best described by the Lennard-Jones potential. As of now, we have not computed the corresponding coefficients $a^{(\alpha, \beta)}$ which would be needed for a more detailed discussion of the theories' agreement to experiments.

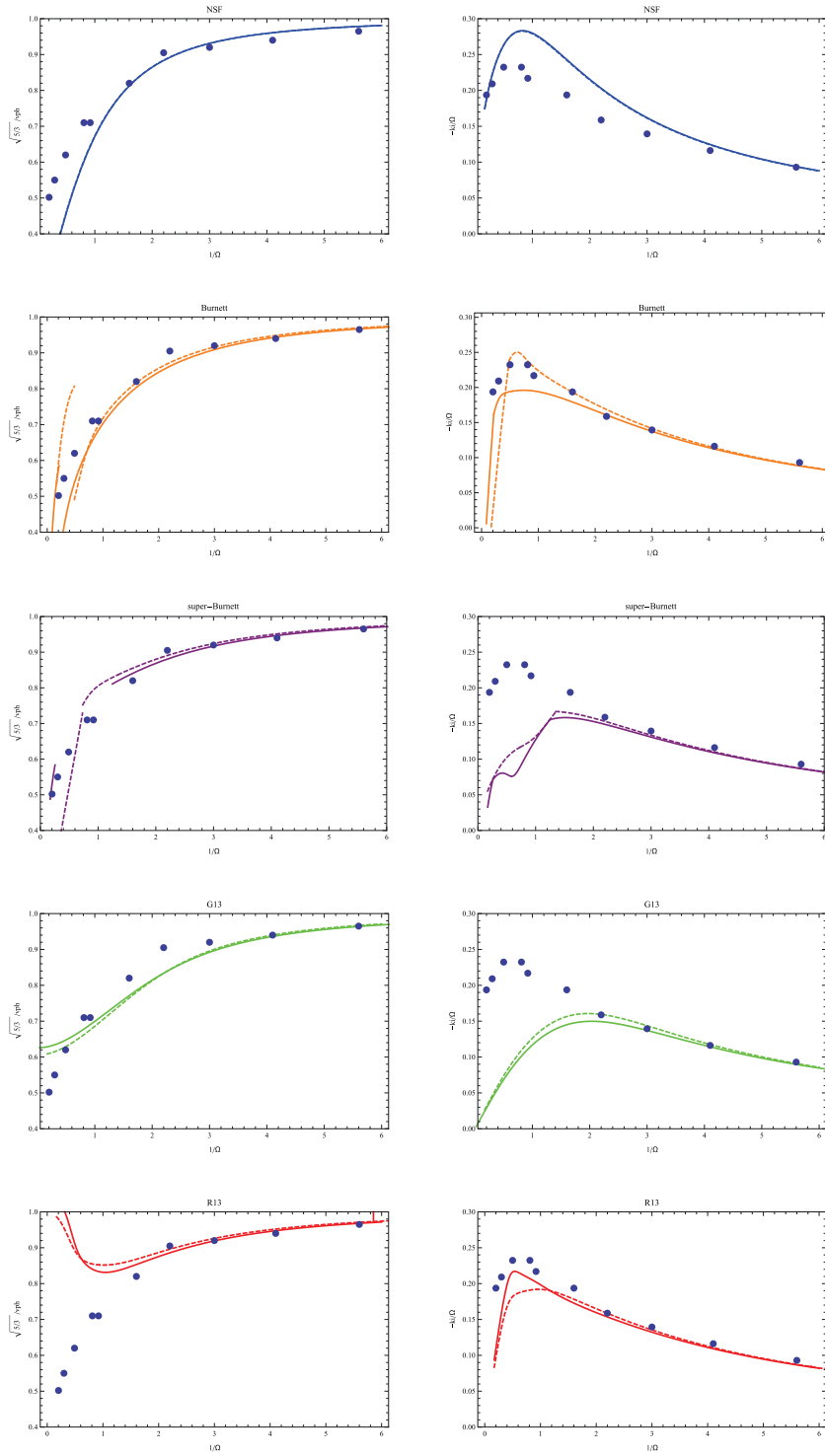


FIGURE 1. Inverse dimensionless phase velocity $\sqrt{5/3}v_{ph}$ (left) and reduced damping $(-k_i)/\omega$ (right) as functions of inverse frequency $1/\omega$ for various theories of extended hydrodynamics: Navier-Stokes-Fourier, Burnett, super-Burnett, Grad13, and R13. Dashed lines are for Maxwell molecules, continuous lines are for hard sphere molecules; dots are measurements for argon [29].

BOUNDARY CONDITIONS

For the original regularized 13-moment equations boundary conditions have been derived and discussed in [9]. They are based on Maxwell's accommodation model for the wall [3], which gives the incoming particles as a superposition of specularly reflected particles and accommodated particles which follow a given wall distribution function.

We choose a wall normal \mathbf{n} corresponding to the velocity component C_n . We denote by f_{wall} the distribution function of the wall and f_{gas} the distribution of the gas just in front of the wall. The distribution function \bar{f} at the wall in the frame of reference of the gas is then given by the accommodation model and reads

$$\bar{f}(\mathbf{C}) = \begin{cases} \chi f_{\text{wall}}(\mathbf{C}) + (1 - \chi) f_{\text{gas}}(\mathbf{C}^*) & C_n > 0 \\ f_{\text{gas}}(\mathbf{C}) & C_n < 0 \end{cases} \quad (11)$$

where the velocity reflection \mathbf{C}^* inverts the sign of the component normal to the wall C_n . According to [9] sensible boundary conditions for the regularized 13-moment equations consider moments of (11) which are odd in the velocity component C_n , i.e., tensors that have an odd number of normal indices when written in the coordinate system of the wall. Let us assume such a moment follows from integration of $\Psi(\mathbf{C})$ which is hence odd in C_n . Integration of both sides of (11) in the frame of the gas and a change of integration $\mathbf{C}^* \leftrightarrow \mathbf{C}$ yields

$$\int_{-\infty}^{\infty} \Psi(\mathbf{C}) \bar{f}(\mathbf{C}) dC_n = \int_{-\infty}^0 \Psi(\mathbf{C}) f_{\text{gas}}(\mathbf{C}) dC_n - (1 - \chi) \int_{-\infty}^0 \Psi(\mathbf{C}) f_{\text{gas}}(\mathbf{C}) dC_n + \chi \int_0^{\infty} \Psi(\mathbf{C}) f_{\text{wall}}(\mathbf{C}) dC_n \quad (12)$$

where we display only the integration with respect to C_n for simplicity. The first integral cancels with the first part of the second term. If we use the decomposition $f_{\text{gas}} = f_{\text{gas}}^{(\text{odd})} + f_{\text{gas}}^{(\text{even})}$ with respect to C_n we can write

$$\int_{-\infty}^0 \Psi(\mathbf{C}) f_{\text{gas}}(\mathbf{C}) dC_n = \frac{1}{2} \int_{-\infty}^{\infty} \Psi(\mathbf{C}) f_{\text{gas}}^{(\text{odd})}(\mathbf{C}) dC_n - \int_0^{\infty} \Psi(\mathbf{C}) f_{\text{gas}}^{(\text{even})}(\mathbf{C}) dC_n \quad (13)$$

where we used the fact that Ψ is odd in C_n . This fact also implies that we can drop the superscript in the first integral in (13) and integrate the complete f_{gas} , again. In (12) we now replace f and f_{gas} by the regularized 13-moment distribution function f_{R13} assuming that this function models both the gas distribution and the distribution at the boundary. We finally transform the integration of the wall distribution f_{wall} into the wall frame with velocity \mathbf{C}_W , assuming the wall does not move in the direction of \mathbf{n} . The final expression reads

$$\int_{\mathbb{R}^3} \Psi(\mathbf{C}) f_{\text{R13}}(\mathbf{C}) d\mathbf{C} = \frac{2\chi}{2 - \chi} \left(\int_0^{\infty} \int_{\mathbb{R}^2} \Psi(\mathbf{C}_W - \mathbf{V}) f_{\text{wall}}(\mathbf{C}_W) dC_t dC_n - \int_0^{\infty} \int_{\mathbb{R}^2} \Psi(\mathbf{C}) f_{\text{R13}}^{(\text{even})}(\mathbf{C}) dC_t dC_n \right) \quad (14)$$

where C_t contain the velocity components tangential to the wall. Following [9] we choose $\Psi(\mathbf{C}) \in \{C_{(n}C_t), C^2C_n, C^2C_{(n}C_t), C_{(n}C_nC_n)\}$ and the R13 distribution function for hard spheres follows from a general Grad distribution where the higher moments are replaced by the leading order constitutive results of the order-of-magnitude method. The impermeability condition of the wall gives the density of the wall distribution f_{wall} .

We will use $V_t = v_t - v_t^{(W)}$ for the slip velocity at the wall and $\Delta\theta = \theta - \theta_W$ for the temperature jump. With this the general boundary condition for a gas described by regularized 13-moment equations in dimensionless formulation are

$$\sigma_{tn} = \beta \left(b^{(1,0)} V_t + b^{(1,1)} q_t - b^{(1,2)} \varepsilon \frac{\partial \sigma_{tn}}{\partial x_n} - b^{(1,3)} \varepsilon \frac{\partial \sigma_{tk}}{\partial x_k} + b^{(1,4)} \Delta q_t \right) \quad (15)$$

$$q_n = \beta \left(b^{(2,0)} \Delta\theta + b^{(2,1)} \sigma_{nn} - b^{(2,2)} \varepsilon \frac{\partial q_{(n}}{\partial x_n} - b^{(2,3)} \varepsilon \frac{\partial q_k}{\partial x_k} - b^{(2,4)} \Delta \sigma_{nn} \right) \quad (16)$$

as generalized slip and jump conditions, and

$$\varepsilon \frac{\partial q_{(t}}{\partial x_n} + b^{(3,5)} \Delta \sigma_{tn} = \beta \left(b^{(3,0)} V_t - b^{(3,1)} q_t + b^{(3,2)} \varepsilon \frac{\partial \sigma_{tn}}{\partial x_n} - b^{(3,3)} \varepsilon \frac{\partial \sigma_{tk}}{\partial x_k} + b^{(3,4)} \Delta q_t \right) \quad (17)$$

$$\varepsilon \frac{\partial \sigma_{nn}}{\partial x_n} = \beta \left(b^{(4,0)} \Delta \theta - b^{(4,1)} \sigma_{nn} + b^{(4,2)} \varepsilon \frac{\partial q_{(n}}{\partial x_n} - b^{(4,3)} \varepsilon \frac{\partial q_k}{\partial x_k} + b^{(4,4)} \Delta \sigma_{nn} \right) \quad (18)$$

as boundary conditions for higher order moment fluxes. The accommodation coefficient is absorbed into the factor $\beta = \chi / (2 - \chi) \sqrt{2/\pi}$ and we are using the abbreviations Δq_i and $\Delta \sigma_{ij}$, see (4). The coefficients $b^{(l,m)}$ can be read off Table 3 for Maxwell molecules and hard spheres, respectively. In comparison to the boundary conditions based on Maxwell molecules not only the coefficients changed, but also some new terms arise..

TABLE 3. Burnett and super-Burnett coefficients for Maxwell molecules and Hard Spheres.

| | MM | HS | | MM | HS | | MM | HS | | MM | HS |
|-------------|-----|---------|-------------|---------|---------|-------------|---------|---------|-------------|---------|---------|
| $b^{(1,0)}$ | 1.0 | 1.0 | $b^{(2,0)}$ | 2.0 | 2.0 | $b^{(3,0)}$ | 0.20833 | 0.12539 | $b^{(4,0)}$ | 0.2 | 0.20770 |
| $b^{(1,1)}$ | 0.2 | 0.20521 | $b^{(2,1)}$ | 0.5 | 0.41802 | $b^{(3,1)}$ | 0.45833 | 0.47552 | $b^{(4,1)}$ | 0.7 | 0.71067 |
| $b^{(1,2)}$ | 1.0 | 1.03061 | $b^{(2,2)}$ | 0.85714 | 0.87743 | $b^{(3,2)}$ | 0.20833 | 0.09633 | $b^{(4,2)}$ | 0.17143 | 0.17326 |
| $b^{(1,3)}$ | 0.0 | 0.00068 | $b^{(2,3)}$ | 0.8 | 0.73977 | $b^{(3,3)}$ | 0.0 | 0.00299 | $b^{(4,3)}$ | 0.08 | 0.07683 |
| $b^{(1,4)}$ | 0.0 | 0.00352 | $b^{(2,4)}$ | 0.0 | 0.07219 | $b^{(3,4)}$ | 0.0 | 0.01784 | $b^{(4,4)}$ | 0.0 | 0.01406 |
| | | | | | | $b^{(3,5)}$ | 0.0 | 0.08057 | | | |

SHEAR FLOW RESULTS

We will briefly demonstrate the effect of different molecule models with the case of rarefied shear flows, in particular, planar Couette flow and acceleration driven Poiseuille flow. In both flows we assume $\mathbf{v} = (v_x(y), 0, 0)$ for the velocity and solve the regularized 13-moment equations (1)-(3). Of special interest in these flows is the parallel heat flow which can be viewed as a rarefaction effect because it arises without temperature gradient.

The solution for Couette flow reads

$$v_x(y) = -\frac{C_0}{\varepsilon} y - \frac{a^{(1,1)} - a^{(1,2)}}{2a^{(1,0)}} q_x(y), \quad q_x(y) = C_1 \sinh\left(\lambda \frac{y}{\varepsilon}\right) \quad (19)$$

for velocity and parallel heat flux. The Poiseuille solution with dimensionless force F follows analogously and is given by

$$v_x(y) = \frac{C_0}{a^{(1,0)}} - \frac{F}{2\varepsilon} y^2 - \frac{a^{(1,1)} - a^{(1,2)}}{2a^{(1,0)}} q_x(y), \quad q_x(y) = -\varepsilon \frac{a^{(2,1)}}{a^{(2,0)}} F + C_1 \cosh\left(\lambda \frac{y}{\varepsilon}\right) \quad (20)$$

In both solutions the Knudsen layer eigenvalue is $\lambda = \sqrt{2a^{(1,0)}a^{(2,0)} / (a^{(1,0)}a^{(2,3)} - a^{(2,2)}(a^{(1,1)} - a^{(1,2)}))}$ which is $\lambda_{MM} = 0.74536$ for Maxwell molecules and $\lambda_{HS} = 0.80703$ for hard spheres. The integration constants $C_{0,1}$ follow from the boundary conditions (15) and (17).

The comparison of the fields is shown in Fig. 2 for $\varepsilon = 0.2$. We use $v_W = 0.1$ in the Couette case and $F = 0.1$ in the Poiseuille case and the accommodation coefficient $\chi = 1$. The molecule model influences the velocity field only weakly, somewhat stronger for Poiseuille. However, the parallel heat flux shows strong quantitative deviations between the Maxwell molecule and hard sphere result. In the future these results will be compared to careful DSMC or direct Boltzmann solutions to verify the new regularized 13-moment equations for hard spheres.

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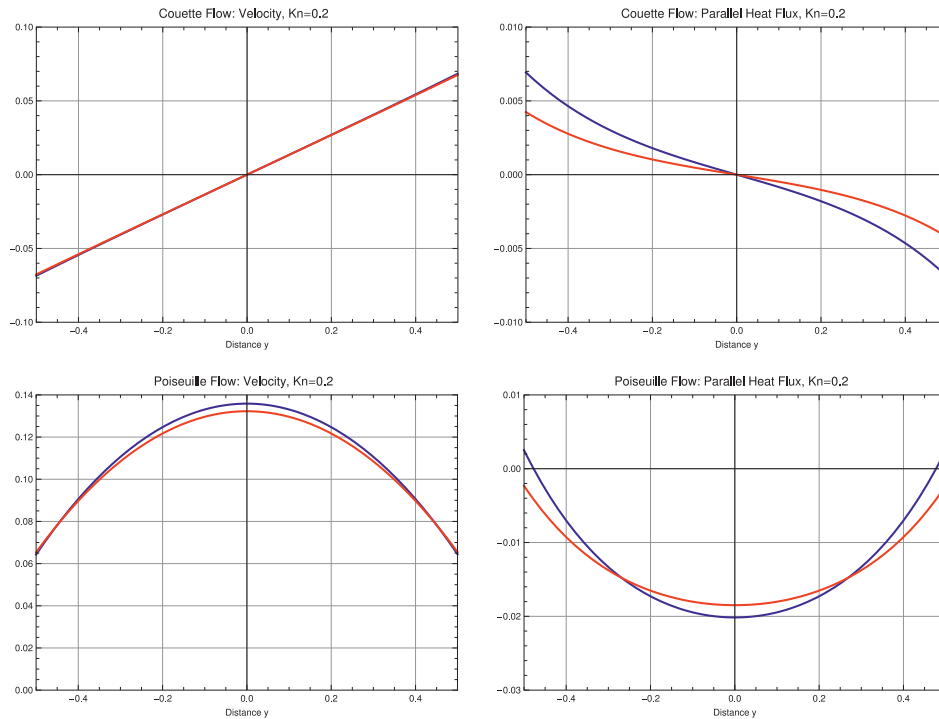


FIGURE 2. Comparison of the R13-results with Maxwell molecules (blue) and hard spheres (red) for classical shear flows. The Couette-flow uses the boundary velocity $v_W = 0.1$. The Poiseuille-flow is driven by a dimensionless acceleration of $F = 0.1$.

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