Numerical Solutions For The BGK-Model With Velocity-Dependent Collision Frequency

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Abstract. The BGK-model with velocity dependent collision frequency is discussed and applied to Couette flow and the shock structure problem. Thermal conductivity and viscosity are computed from the Chapman-Enskog method and several velocity-dependent collision frequencies are introduced which all give the proper Prandtl number. The models are tested and compared to results from the Direct Simulation Monte Carlo method. The simulations rely on a numerical scheme that ensures positivity of solutions, conservation of moments, and dissipation of entropy. The advantages and disadvantages of the various BGK models are discussed.

INTRODUCTION

Because of its simplicity compared to the Boltzmann equation the BGK equation is widely used in the kinetic theory of gases [1]. While the BGK equation gives qualitatively good results, it fails when one is interested in quantitatively correct results. This fact manifests itself most prominently in the computation of the Prandtl number, i.e. the ratio of thermal conductivity κ and viscosity μ. While measurements and the theory of the full Boltzmann equation give $Pr \simeq \frac{2}{3}$, one obtains $Pr = 1$ from the standard BGK model [2].

There are two main approaches to modify the BGK model in order to obtain the proper Prandtl number, the ellipsoidal statistical model (ES- BGK model)[3][4], and the BGK-model with velocity dependent collision frequency ($\nu(C)$-BGK model)[5][6]. In all three approaches, standard BGK, ES-BGK, and $\nu(C)$-BGK, the Boltzmann collision term is replaced by a relaxation type term of the general form

$$S_{BGK} = -\nu(f - f_E)$$

where ν is the collision frequency, f is the actual distribution function of the microscopic velocities of the gas, and f_E is a suitable equilibrium phase density. In standard and ES-BGK model, the collision frequency is a constant to be fitted to viscosity data, but in the standard BGK model f_E is the local Maxwell distribution f_M, i.e. an isotropic Gaussian, while in the ES-BGK model f_E is a local anisotropic Gaussian. In the $\nu(C)$-BGK model ν is a function of the microscopic velocity C of the particles and f_E is a local isotropic Gaussian, albeit not the local Maxwellian.

The BGK model with velocity-dependent collision frequency is briefly discussed in the book of Cercignani [2], and Bouchut and Perthame discussed it thoroughly from a mathematical viewpoint [5]. To our knowledge, the first attempt to consider an explicit expression for $\nu(C)$ can be found in [6] where the simplest possible ansatz, namely $\nu(C) \sim C^n$ was considered. Here, we present some alternative functions for the collision frequency and solve the corresponding BGK equation for Couette flow and the shock structure problem. The results will be compared with solutions obtained from the standard and the ES-BGK models, and with Monte Carlo computations.

The numerical method used for solving the various BGK equations considered here, is the method by Mieussens [7][8][9]. The great advantage of this method compared to others is that it guarantees the conservation of mass, momentum, and energy.

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BGK MODELS

The goal of kinetic theory is to find the the phase density f, defined such that $f d\mathbf{c}$ gives the number density of atoms with velocity in $(c_i, c_i + dc_i)$ at place x_i and time t. The macroscopic quantities density ρ, velocity v_i, density of internal energy $\rho\varepsilon$, pressure tensor $p_{\langle ij\rangle}$ and heat flux vector q_i of the gas are given by moments of the phase density, viz.

$$\rho = m\int f d\mathbf{c}\ ,\ \ \rho v_i = m\int c_i f d\mathbf{c}\ ,\ \ \rho\varepsilon = \frac{3}{2}\rho\frac{k}{m}T = \frac{m}{2}\int C^2 f d\mathbf{c} \tag{1}$$
$$p_{\langle ij\rangle} = m\int C_{\langle i}C_{j\rangle} f d\mathbf{c}\ ,\ \ q_i = \frac{m}{2}\int C^2 C_i f d\mathbf{c}$$

where m is the mass of one particle, k is Boltzmann's constant, and $C_i = c_i - v_i$ is the peculiar velocity; T is the gas temperature, defined by Eqn. $(1)_3$. The entropy of the gas is given by

$$\rho s = -k\int f \ln f d\mathbf{c}.$$

The phase density $f(x_i, t, c_i)$ is governed by the Boltzmann equation [2]

$$\frac{\partial f}{\partial t} + c_i\frac{\partial f}{\partial x_i} = S\ . \tag{2}$$

Because of its complex non-linearity, the Boltzmann collision term S is difficult to handle. Therefore one is interested in model equations which should have the same properties as the original equation. In the BGK model, the collision term is replaced by

$$S_\gamma = -\nu\left(f - f_\gamma\right) \tag{3}$$

where f_γ is of the form, see [10][6][11],

$$f_\gamma = a\exp\left(-\Gamma C^2 + \gamma_i C_i\right)\ . \tag{4}$$

The coefficients a, Γ, γ_i for the distribution (4) follow from the conservation conditions for mass, momentum and energy

$$\int \nu m\left(f - f_\gamma\right) d\mathbf{c} = 0\ ,\ \ \int \nu m C_i\left(f - f_\gamma\right) d\mathbf{c} = 0\ ,\ \ \int \nu\frac{m}{2}C^2\left(f - f_\gamma\right) d\mathbf{c} = 0\ . \tag{5}$$

Note, that f_γ is only a Maxwellian if ν does not dependent on the peculiar velocity C_i.

We proceed to discuss the properties of the BGK model which are the same ones as those of the original Boltzmann equation:

i.) Conservation of mass, momentum and energy is ensured by the proper choice of a, Γ, γ_i according to Eqns. (5)

ii.) Since, with (5),

$$k\int \ln f_\gamma S_\gamma d\mathbf{c} = k\int\left(\ln a - \Gamma c^2 + \gamma_i c_i\right) S_\gamma d\mathbf{c} = 0$$

we obtain the positivity of the entropy production (H-theorem)

$$-k\int \ln f S_\gamma d\mathbf{c} = -k\int \ln f S_\gamma d\mathbf{c} + k\int \ln f_\gamma S_\gamma d\mathbf{c} = k\int \nu \ln\frac{f}{f_\gamma}\left(f - f_\gamma\right) d\mathbf{c} \geqslant 0\ .$$

iii.) In thermodynamic equilibrium (characterized by the subscript E) the BGK collision term vanishes

$$S_{|E} = 0 \Longrightarrow -\nu\left(f_{|E} - f_{\gamma|E}\right) = 0,$$

i.e. in equilibrium both phase densities are equal, $f_{|E} = f_{\gamma|E}$. This implies that both functions have the same moments. Since the first five moments of f define density, velocity and temperature, we conclude that both functions are Maxwellians

$$f_{|E} = f_{\gamma|E} = f_M = \frac{\rho}{m}\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}\exp\left[-\frac{mC^2}{2kT}\right]$$

iv.) The extension of the ordinary BGK model to the case where ν is a function of C offers an additional degree of freedom which may be used to adjust both, viscosity and thermal conductivity, to their measured values so that the proper Prandtl number results. The details will be discussed below.

In summary, we conclude that the BGK model with a velocity-dependent collision frequency may be formulated so as to have the same properties i.)-iv.) as the Boltzmann equation.

The BGK equation follows from (2) after replacement of S by S_γ. We proceed by approximating the phase density f by means of the Chapman-Enskog method [2] in order to compute viscosity and heat conductivity. The first order Chapman-Enskog expansion relies on the assumption that the phase density is close to a Maxwellian, i.e. $f \simeq f_M(1+\phi)$, where $\phi \ll 1$. Then, the equilibrium distribution f_γ will be close to equilibrium as well, so that $f_\gamma = f_M\left(1+\phi_\gamma\right)$ with $\phi_\gamma \ll 1$. In fact, we can write

$$f_\gamma = \frac{\rho}{m}\sqrt{\frac{m}{2\pi kT}}^3 (1-\hat{a})\exp\left[-\left(\frac{m}{2kT}-\hat{\Gamma}\right)C^2+\gamma_i C_i\right] \simeq f_M\left[1-\hat{a}+\hat{\Gamma}C^2+\gamma_i C_i\right]$$

where the coefficients $\hat{a}$, γ_i, $\hat{\Gamma}$ measure the deviation from the Maxwellian and are assumed to be small. We insert the Maxwell phase density on the right hand side of the BGK equation and eliminate all time derivatives by means of the Euler equations for monatomic gases, to find the phase density as

$$f = f_\gamma - \frac{1}{\nu} f_M\left\{\frac{m}{kT}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}C_{\langle i}C_{j\rangle} + \frac{1}{T}\frac{\partial T}{\partial x_i}\left(\frac{m}{2kT}C^2-\frac{5}{2}\right)C_i\right\}. \tag{6}$$

This approximate solution fulfills the conservation conditions (5) for *any* distribution f_γ so that the coefficients $\hat{a}$, γ_i, $\hat{\Gamma}$ cannot be determined from these conditions. However, the phase density (6) must reproduce the first moments $(1)_{1-3}$ and it follows that $\hat{a} = \hat{\Gamma} = 0$ and

$$\gamma_i = \frac{8}{3\sqrt{\pi}}\frac{1}{T}\frac{\partial T}{\partial x_i}\int \frac{\eta^4\left(\eta^2-\frac{5}{2}\right)}{\nu(\eta)}e^{-\eta^2}d\eta$$

where $\eta = \sqrt{\frac{m}{2kT}}C$. Now it is an easy task to calculate the pressure deviator $p_{\langle ij\rangle}$ and the heat flux vector q_i. Of course, we find the laws of Navier-Stokes and Fourier with explicit expressions for viscosity μ and thermal conductivity κ, viz.

$$p_{\langle ij\rangle} = -\underbrace{\frac{32}{15\sqrt{\pi}}\rho\frac{k}{m}T\int\frac{\eta^6}{\nu(\eta)}e^{-\eta^2}d\eta}_{2\mu}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \quad , \quad q_i = -\underbrace{\frac{8}{3\sqrt{\pi}}\rho\frac{k^2}{m^2}T\int\frac{\eta^4\left(\eta^2-\frac{5}{2}\right)^2}{\nu(\eta)}e^{-\eta^2}d\eta}_{\kappa}\frac{\partial T}{\partial x_i} \tag{7}$$

As expected, the Prandtl number depends on the collision frequency

$$Pr = \frac{5}{2}\frac{k}{m}\frac{\mu}{\kappa} = \int\frac{\eta^6}{\nu(\eta)}e^{-\eta^2}d\eta \Big/ \int\frac{\eta^4\left(\eta^2-\frac{5}{2}\right)^2}{\nu(\eta)}e^{-\eta^2}d\eta. \tag{8}$$

There is an infinite number of possible functions $\nu(\eta)$ that give the proper Prandtl number. Since the true collision frequency is an increasing function in η, we consider only increasing functions for which we introduce the notation

$$\nu(\eta) = \frac{\rho\frac{k}{m}T}{\mu}\hat{\nu}(\eta) \quad \text{with} \quad \frac{16}{15\sqrt{\pi}}\int\frac{\eta^6}{\hat{\nu}(\eta)}e^{-\eta^2}d\eta = 1\,. \tag{9}$$

Four simple dimensionless collision frequencies that all give $Pr = 2/3$ are

$$\hat{\nu}_1(\eta) = 0.431587\,\eta^{1.791288}\,, \qquad \hat{\nu}_2(\eta) = 0.0268351\left(1+14.2724\eta^2\right)\,,$$
$$\hat{\nu}_3(\eta) = 0.0365643\left(1+10\eta^{2.081754}\right)\,, \quad \hat{\nu}_4(\eta) = 0.1503991\left(1+0.92897\eta^4\right)\,.$$

In the case of hard sphere molecules, one finds $\hat{\nu}_{HS}(0) = 0.557608$ for molecules at rest and $\hat{\nu}_{HS}(\eta \gg 1) = 0.4941673\,\eta$ for fast particles [12]. Thus, in comparison to hard sphere molecules, our models underestimate the collision frequency for slower particles and overestimate that of faster particles.

NUMERICAL METHOD

For the sake of simplicity, our numerical method is presented in one spatial dimension, but three dimensions in velocity, see [9, 8] for a complete description. The equation to be approximated is

$$\frac{\partial f}{\partial t} + c_x \frac{\partial f}{\partial x} = -\nu(f - f_\gamma), \qquad 0 \le x \le L. \tag{10}$$

The space variable x is discretized on a uniform grid defined by nodes $x_i = i\Delta x$ with $x_0 = 0$ and $x_I = L$. The velocity c_x is discretized by nodes $c_x^{(j_1)} = c_{x,min} + j_1 \Delta c_x$, with $c_x^0 = c_{x,min}$ and $c_x^{J_1} = c_{x,max}$; c_y and c_z are discretized accordingly. For brevity, we write $c_j = (c_x^{(j_1)}, c_y^{(j_2)}, c_z^{(j_3)})$ where $j = (j_1, j_2, j_3)$. Finally, time is discretized as $t_n = n\Delta t$.

Eqn. (10) is then classically approximated by a finite volume scheme,

$$f_{i,j}^{n+1} = f_{i,j}^n - \frac{\Delta t}{\Delta x}(F^{\,n}_{i+\frac{1}{2},j} - F^{\,n}_{i-\frac{1}{2},j}) - \Delta t\, \nu_{i,j}^n (f_{i,j}^n - f_{\gamma,i,j}^n), \tag{11}$$

where the above quantities are defined as follows:

- $f_{i,j}^n$ is an approximation of $f(x_i, t_n, c_j)$;
- numerical fluxes are defined by

$$F^{\,n}_{i+\frac{1}{2},j} = \frac{1}{2}\left(c_x^{(j_1)} (f_{i+1,j}^n + f_{i,j}^n) - |c_x^{(j_1)}| (\Delta f^n_{i+\frac{1}{2},j} - \Phi^n_{i+\frac{1}{2},j}) \right),$$

  with the notation $\Delta f^n_{i+\frac{1}{2},j} = f^n_{i+1,j} - f^n_{i,j}$, and the flux limiter function $\Phi^n_{i+\frac{1}{2},j}$ allows to obtain a second order scheme, $\Phi^n_{i+\frac{1}{2},j} = 0$ for first order, and $\Phi^n_{i+\frac{1}{2},j} = \text{minmod}(\Delta f^n_{i-\frac{1}{2},j}, \Delta f^n_{i+\frac{1}{2},j}, \Delta f^n_{i+\frac{3}{2},j})$ for second order;
- the collision frequency is defined by

$$\nu_{i,j}^n = \frac{\rho_i^n \frac{k}{m} T_i^n}{\mu(T_i^n)} \hat{\nu}(\eta_{i,j}^n), \qquad \text{with } \eta_{i,j}^n = \sqrt{(c_x^{(j_1)} - v_i^n)^2 + (c_y^{(j_2)})^2 + (c_z^{(j_3)})^2} \Big/ \sqrt{2\frac{k}{m} T_i^n};$$

- macroscopic quantities are defined as in Eqn. (1) where now continuous integrals are replaced by discrete sums on the velocity grid

$$\left(\rho_i^n, \quad \rho_i^n v_i^n, \quad \tfrac{3}{2}\rho_i^n \tfrac{k}{m} T_i^n\right) = m \sum_{j=(0,0,0)}^{(J_1,J_2,J_3)} \left(1, \quad c_x^{(j_1)}, \quad \left((c_x^{(j_1)} - v_i^n)^2 + (c_y^{(j_2)})^2 + (c_z^{(j_3)})^2\right)\right) f_{i,j}^n \Delta c_x \Delta c_y \Delta c_z,$$

- the approximation of $f_\gamma(x_i, t_n, c_j)$ is defined by

$$f_{\gamma,i,j}^n = a_i^n \exp\left[-\Gamma_i^n \left((c_x^{(j_1)} - v_i^n)^2 + (c_y^{(j_2)})^2 + (c_z^{(j_3)})^2 \right) + \gamma_i^n (c_x^{(j_1)} - v_i^n) \right],$$

  where the three coefficients $a_i, \Gamma_i^n, \gamma_i^n$ are solutions of the discrete version of Eqn. (5) that are solved by a Newton algorithm.

Owing to this last approximation, our scheme is perfectly conservative for density, momentum, and total energy. Moreover, the positivity of the phase density is preserved, if at each iteration the time step follows the condition

$$\Delta t \left(\max_{i,j} \nu_{i,j}^n + \max_j \frac{|c_x^{(j_1)}|}{\Delta x} \right) < 1, \tag{12}$$

also the total entropy is increasing.

For the computation of steady states, condition (12) is very restrictive for dense or rapid regimes where Δt is small and the convergence is very slow. A classical way to overcome this difficulty is to use a linearized implicit scheme,

$$f_{i,j}^{n+1} + \frac{\Delta t}{\Delta x}(F^{\,n+1}_{i+\frac{1}{2},j} - F^{\,n+1}_{i-\frac{1}{2},j}) + \Delta t\, \nu_{i,j}^n (f_{i,j}^{n+1} - f_{\gamma,i,j}^{n+1}) = f_{i,j}^n.$$

Since $f_{\gamma,i,j}^{n+1}$ is a non-linear function of $f_{i,j}^{n+1}$, it is linearized as

$$f_{\gamma,i,j}^{n+1} \approx f_{\gamma,i,j}^{n} + [D_i^n (f_i^{n+1} - f_i^n)]_j,$$

where D_i^n is the Jacobian of the mapping $g \mapsto f_\gamma[g]$ evaluated at f_i^n. For the second order scheme, the flux limiters (non differentiable) are kept explicit. The following δ matrix-form of the scheme is more adapted to computations

$$\left(\frac{I}{\Delta t} + T + R^n\right) \delta f^n = RHS^n, \tag{13}$$

where $\delta f^n = f^{n+1} - f^n$, I is the unit matrix, T is a matrix such that $(T f^n)_{i,j} = \frac{1}{\Delta x}(F^{\,n}_{i+\frac{1}{2},j} - F^{\,n}_{i-\frac{1}{2},j})$ with only the first order fluxes, R^n is such that $(R^n f^n)_{i,j} = \nu_{i,j}^n (f_{i,j}^n - [D_i^n f_i^n]_j)$, and

$$RHS_{i,j}^n = -\frac{1}{\Delta x}(F^{\,n}_{i+\frac{1}{2},j} - F^{\,n}_{i-\frac{1}{2},j}) - \nu_{i,j}^n (f_{i,j}^n - f_{\gamma,i,j}^n) \tag{14}$$

which contains the limiters for the second order scheme.

The scheme now reads as a linear system to be solved at each iteration. This can be done efficiently, and this method has been proved to be very fast for computing steady flows. This scheme theoretically preserves conservation of mass, momentum and total energy, but it should be noted that the linear system (14) is never solved directly. Instead, an iterative method is used. It is known in CFD that convergence of such an iterative method is not required for the global convergence towards the steady state. However, the iterative solver must be carefully chosen so as to preserve conservation properties.

NUMERICAL RESULTS

In the continuum regime, i.e. for Knudsen numbers below 0.01, the flow is expected to be well described by the Navier-Stokes-Fourier equations. Since both models, $\nu(C)-$BGK and ES-BGK, are constructed such that they have proper viscosity and heat conductivity in the continuum regime, numerical simulations for small Knudsen numbers show only small differences between the different corrected BGK models, and the results match well with solutions of the Navier Stokes equations [11].

In the transition regime, i.e. for Knudsen numbers between 1 and 0.01, Knudsen number effects are expected to be visible. These include, but are not limited to, jumps in temperature and velocity slip at the walls.

As a test case we consider one-dimensional plane Couette flow of argon in the transition regime, similar to a testcase of Bird [13]: the gas is confined between two plates maintained at $T_w = T_0 = 273$ K, the distance between the plates being $L = 1$m. One plate is at rest while the other is moving in y direction with velocity $u_w = 300$ m/s. Initially, the gas is at T_0, and its density is $\rho_0 = 9.28 \times 10^{-7}$ kg/m^3, corresponding to a pressure $p_0 = \rho_0 \frac{k}{m} T_0 = 0.0528\,$Pa. The viscosity of the gas is given by $\mu(T) = \mu_0 (T/T_0)^\omega$ with $\mu_0 = 2.117 \times 10^{-5} \frac{kg}{ms}$ and $\omega = 0.81$, corresponding to $Kn = \frac{\mu}{p}\sqrt{\frac{\pi}{2}\frac{kT}{m}} = 0.1199$.

For the numerical calculations, we use a grid of 200 cells in x direction and $13 \times 17 \times 13$ discrete velocities with bounds $[-913, 913] \times [-1253, 1253] \times [-913, 913]$ (in m/s), for further details on the numerics see [11].

Figure 1 shows profiles for density, temperature, velocity, heat flux and stress tensor for standard BGK model, ES-BGK model, and the $\nu(C)$-BGK models $\hat{\nu}_1(\eta), \hat{\nu}_2(\eta), \hat{\nu}_3(\eta)$. The collision frequency $\hat{\nu}_4(\eta)$ is not considered, since its maximum value is so large that by Eqn. (12) the corresponding time step becomes forbiddingly small. For comparison, we use results from the DSMC method with variable hard sphere model [13].

For density, curves obtained with the $\nu(C)-$BGK models are close to the DSMC curves in the interior ($0.2 \le x \le 0.8$), and results obtained with standard BGK and ES models are close together and differ considerably from DSMC in the interval $0.4 \le x \le 0.6$. For temperature, however, the ES model is closest to DSMC, and the temperature jumps at the boundaries of standard BGK and ES models ($\Delta T_W = 9K$) are closer to those of the DSMC ($\Delta T_W = 8.4K$) than those of the $\nu(C)-$ BGK model ($\Delta T_W = 9.5K$). Similar behavior is observed for velocity slip. For shear stress, however, the $\nu(C)-$BGK models with ν_2, ν_3 lie closest to DSMC, surprisingly all models agree on the heat flux.

As a second test case we consider the shock structure for a one-dimensional steady shock with an upstream Mach number of 8 in argon, one of the reference problems in [13]. The details of the shock structure depend strongly on the details of the microscopic interaction, which are reflected in the velocity dependence of the collision frequency.

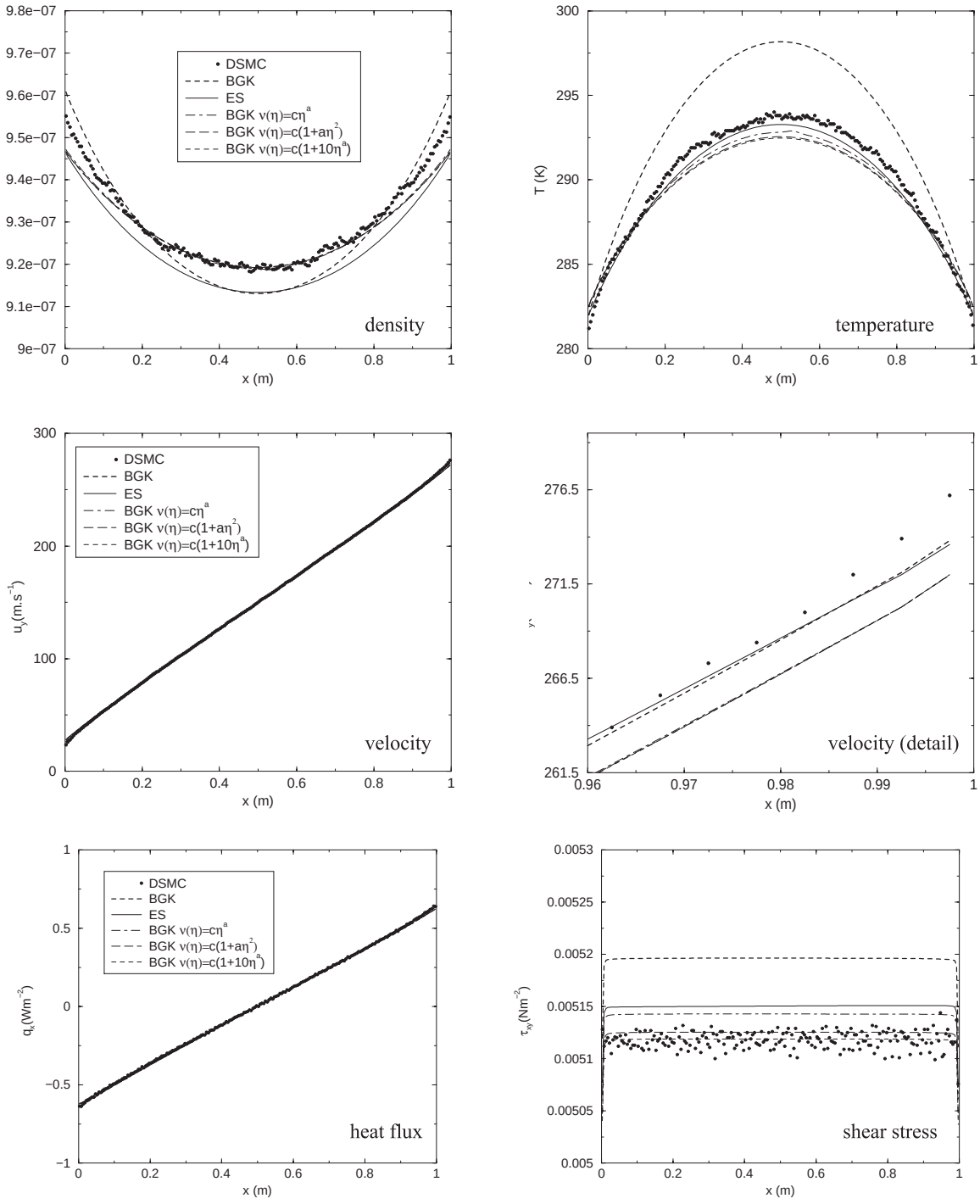

FIGURE 1. Couette flow, profiles for wall velocity $u_w = 300$ m/s and Knudsen number 0.1199.

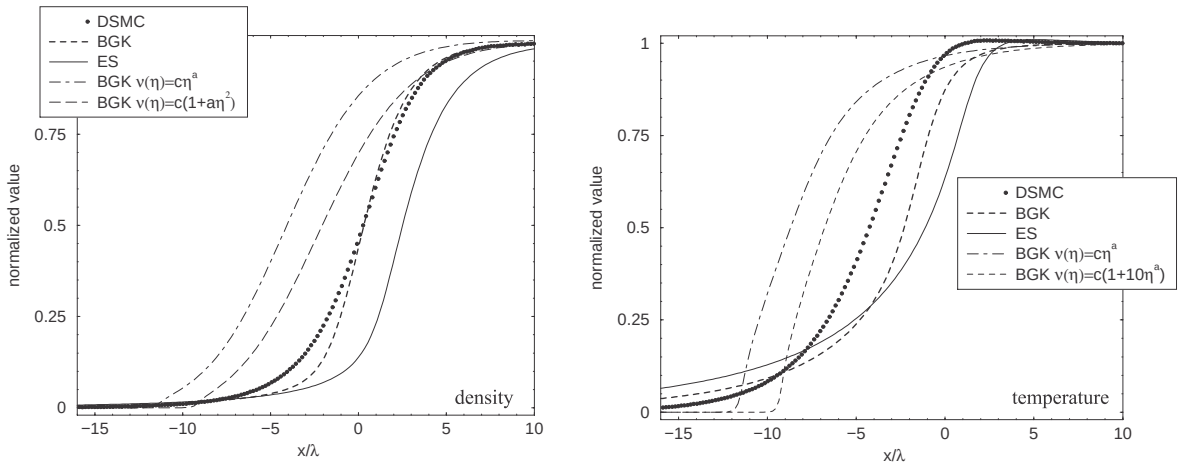

FIGURE 2. Density and temperature profiles for a stationary shock at Mach 8.

Figure 2 shows the profiles of density and temperature of the shock for our models. Clearly, the standard BGK and the ES-BGK model give density curves close to the DSMC, while the $\nu(C)$-BGK models give a flatter profile. However, the temperature profiles in Figure 2 are too steep for the $\nu(C)$-BGK models, and too flat for standard BGK, and ES-BGK. Only the ES-BGK model gives a overshoot in the temperature curve similar to that seen in the DSMC result.

CONCLUSIONS

From our results for Couette flow and shock structure, we draw the following conclusions:

i.) In the continuum regime ($Kn < 0.01$) all BGK models with correct viscosity and heat conductivity, that is $\nu(C)$-BGK and ES-BGK, give identical results in agreement with the Navier-Stokes-Fourier equations. Here, the $\nu(C)$-BGK model is in disadvantage to the ES-BGK model, since it requires a smaller time step. This can be seen from Eqn. (12) which relates the time step to the maximum value of the collision frequency. The maximum value $\nu(C_{\max})$ of the $\nu(C)$-BGK models are larger than the constant collision frequency of the ES-BGK model, so that the latter allows larger time steps, and therefore faster numerical calculations.

ii.) When microscale effects become important, i.e. at Knudsen numbers above 0.01 or in shocks, all BGK-type models considered here lead to different results. The ES-BGK model is numerically cheapest, and we can say that it gives the best overall performance of the models considered. However, also the ES-BGK model is not capable of making accurate predictions for the transition regime, as becomes most apparent in the density curves of Figure 1 and the temperature profile of Figure 2.

All together, our results show that improved BGK models are accurate in the continuum regime, and can give qualitatively good results in the transition regime. However, they are not capable of an accurate description of microscale effects such as slip, temperature jump and shock structure in agreement with the Boltzmann equation.

Nevertheless, our results indicate that considering the non-isotropic Gaussian in the ES–BGK model, as well as considering velocity dependent collision frequencies in the $\nu(c)$-BGK models lead to considerable improvement over the standard BGK model. We expect that the combination of an anisotropic Gaussian with a velocity dependent collision frequency in a $\nu(C)$-ES-BGK model might give the best results. In such a model, one could use the true collison frequency. The $\nu(C)$-ES-BGK model will be considered in a future paper.

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