A DSMC view of the problem of bulk viscosity in thermal nonequilibrium

D. Bruno

Istituto di Metodologie Inorganiche e dei Plasmi, Consiglio Nazionale delle Ricerche,
via G. Amendola, 122/D, 70125 Bari, Italy

Abstract. Spontaneous fluctuation power spectra in the hydrodynamic regime are obtained from DSMC simulations of a model gas with internal degrees of freedom. The simulated spectra are compared with the theoretical results derived from one-temperature and two-temperature hydrodynamic conservation equations. The comparison allows to establish the limitations of a bulk viscosity description of the internal energy relaxation kinetics.

INTRODUCTION

For a gas possessing internal degrees of freedom, the fluid dynamic equations derived by kinetic theory in conditions of thermal equilibrium show the appearance of bulk viscosity as a consequence of the finite relaxation time of the internal degrees of freedom. The classical Chapman-Enskog treatment results in expressions for the bulk viscosity that is directly proportional to the relaxation time [3]. When the relaxation time is comparable to the flow characteristic time, this theory is not applicable and frequency dependent transport coefficients have been invoked [1]. On the other hand, the two-temperature formalism describes correctly the relaxation of the internal energy content but it does not, apparently, exhibit a bulk viscosity effect [4]. In order to clarify these points, the transport properties of a model molecular gas are studied. The gas is simulated by DSMC and the transport properties are derived by analysis of the thermal fluctuation power spectrum. Results, therefore, do not depend on any assumption for the derivation of the conservation equations from the Boltzmann equation. Comparison of the spectra obtained from DSMC simulations with those obtained from the one-temperature Chapman-Enskog theory show that the latter is adequate for the description of the transport properties of the gas only if the relaxation time for the internal degrees of freedom is small as compared to the flow characteristic time. The spectra derived in the framework of the two-temperature model, instead, describe appropriately the hydrodynamic fluctuations for any value of the internal energy relaxation time. The interest is twofold: first, it is shown that the two-temperature model is the correct generalisation of the one-temperature model. Besides, it is demonstrated how the introduction of frequency dependent transport coefficients in an unnecessary complication. In the following sections, the one-temperature and two-temperature fluid dynamic equations, as obtained from the Chapman-Enskog perturbative solution of the Boltzmann equation are recalled. Next, the procedure to obtain the spontaneous fluctuation spectra is outlined. Then, the model gas is introduced and details are given on the DSMC implementation and on the means to obtain the fluctuation power spectra from the simulations. Finally, results are discussed and some conclusions are drawn.

TRANSPORT PROPERTIES OF DILUTE GASES WITH INTERNAL DEGREES OF FREEDOM

In this sections the flud dynamic equations and the linear closure relations are recalled that can be derived by the Chapman-Enskog method of solution of the Boltzmann equation [3]. In order to simplify the notation, a single gas is considered with a single set of internal energy levels. For this system, kinetic theory introduces different approaches, depending on the hierarchy of characteristic relaxation times. When all internal energy relaxation times are small as compared to a macroscopic flow characteristic time, a one-temperature model can be derived. When, instead, some of the internal energy relaxation times are comparable to the flow characteristic time, multi-temperature approaches are

required. In this respect, a state-to-state description is only a generalisation of the multi-temperature model and it will not be considered.

One-temperature model

For a single gas with a single set of internal energy levels (g_i, ε_i), the fluid dynamic equations in the one-temperature description are [3]:

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} = 0 \tag{1}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot \mathbf{P} = 0 \tag{2}$$

$$\rho \frac{\partial U}{\partial t} + \rho \mathbf{v} \cdot \nabla U + \nabla \cdot \mathbf{q} + \mathbf{P} : \nabla \mathbf{v} = 0 \tag{3}$$

where:

$$U = \frac{3}{2} \frac{k_B T}{m} + \frac{1}{m} \frac{\sum_i g_i \varepsilon_i e^{-\frac{\varepsilon_i}{k_B T}}}{\sum_i g_i e^{-\frac{\varepsilon_i}{k_B T}}}$$

And the closure relations for the fluxes are, in the linear regime:

$$\begin{aligned}
\mathbf{P} &= (p - \mu \nabla \cdot \mathbf{v})\mathbf{I} - 2\eta \mathbf{S} \\
\mathbf{q} &= -\lambda \nabla T
\end{aligned}$$

The transport coefficients that appear in these equations can be evaluated in terms of the collision integrals that describe the average interaction among particles in collision. For Hard Spheres, in the first approximation [3]:

$$\begin{aligned}
\eta &= \frac{5}{16} \frac{\sqrt{\pi m k_B T}}{\sigma} \\
\lambda &= \eta \{ \frac{5}{2} c_{tr} + \frac{\rho \mathscr{D}}{\eta} c_{int} \} \\
\mu &= p \frac{c_{int}}{c_{tr}} \frac{1}{c_{int} + c_{tr}} \tau
\end{aligned}$$

where τ is the internal energy relaxation time.

Two-temperature model

In this case, an additional macroscopic variable is introduced that describes the internal energy content [4]:

$$U_{int} = \frac{1}{m} \frac{\sum_i g_i \varepsilon_i e^{-\frac{\varepsilon_i}{k_B T_{int}}}}{\sum_i g_i e^{-\frac{\varepsilon_i}{k_B T_{int}}}}$$

Equations (1)-(3) are unchanged but now:

$$\begin{aligned}
\mu &= 0 \\
U &= \frac{3}{2} \frac{k_B T}{m} + U_{int} \\
\mathbf{q} &= -\lambda_{tr} \nabla T - \lambda_{int} \nabla T_{int}
\end{aligned}$$

In addition, there is a conservation equation for the internal energy:

$$\rho \frac{\partial U_{int}}{\partial t} + \rho \mathbf{v} \cdot \nabla U_{int} + \nabla \cdot \mathbf{q_{int}} - \dot{u}_{int} = 0 \tag{4}$$

where:

$$\dot{u}_{int} = -\frac{1}{4} \sum \Delta\varepsilon (K_{kl}^{ij} n_k n_l - K_{ij}^{kl} n_i n_j) \tag{5}$$

Spontaneous fluctuations and transport properties

For systems in thermodynamic equilibrium general relations can be derived among the transport properties of the system in the hydrodynamic regime and the space-time correlation functions that describe the spontaneous fluctuations of the macroscopic quantities around the equilibrium values. These relations, being based only on the thermal equilibrium assumption, are independent of the physical assumptions made in deriving the equations governing the evolution of the system. The procedure is therefore the same both for one- and two-temperature models. From the governing equations we derive linearized equations for the fluctuations of the macroscopic variables. These are then doubly Laplace-Fourier transformed to the (k, ω) space. The equations are then solved for $\delta\tilde{\rho}_k(s = \varepsilon + i\omega)$. The latter is used to construct the space time correlation function $< \delta\rho_k^*(0)\delta\tilde{\rho}_k(s) >$. Finally, this correlation function can be connected with the density fluctuation power spectrum $S(k, \omega)$ that is a quantity experimentally measurable in light scattering experiments:

$$\frac{S(k, \omega)}{S(k)} = 2Re \lim_{\varepsilon \to 0} \frac{< \delta\rho_k^*(0)\delta\tilde{\rho}_k(s) >}{< \delta\rho_k^*(0)\delta\rho_k(0) >}$$

The fluctuation power spectrum for the one-temperature model has been derived in [1], whereas that for the two-temperature model has been derived in the present work, limited to the simple case studied and using the zero-order approximation for $\dot{u}_{int}$.

DSMC SIMULATION OF SPONTANEOUS FLUCTUATION SPECTRA

Since DSMC is a Monte Carlo method of solution of the Boltzmann equation, it can be applied to the simulation of the spontaneous fluctuations of a gas mixture. It has previously been shown that DSMC gives correct results for atomic gases both in hydrodynamic and rarefied regimes[2].

In the present case we apply the method to the simulation of the spontaneous fluctuations of a model gas with internal degrees of freedom.

Physical system

A single gas of Hard Spheres is considered with $mass = 28.9641 \, amu$, $\sigma = 7.2 \cdot 10^{-19} \, m^2$. The gas has 2 internal energy levels with weight and energy as detailed below:

$$\begin{aligned} g_0 &= 1, & \varepsilon_0 &= 0 \\ g_1 &= 9, & \varepsilon_1 &= 1000 \, K \end{aligned}$$

Molecules exchange internal energy in collision according to the simplest single-quantum, line-of-centers model:

$$\begin{aligned} p(0 \leftarrow 1) &= p_0 \\ p(1 \leftarrow 0) &= \begin{cases} 0 & E < \varepsilon_1 \\ s_1 p_0 (1 - \frac{\varepsilon_1}{E}) & E \geq \varepsilon_1 \end{cases} \end{aligned}$$

For this simple model all transport properties can be calculated. In particular, in thermal equilibrium ($T = T_{int}$):

$$\dot{u}_{int}^{(0)} = \frac{nc_{int}}{\tau}(T - T_{int})$$

$$\tau^{-1} = nK_1^0(1 + s_1 e^{-\frac{\varepsilon_1}{k_b T}})$$

$$K_1^0 = 4p_0\sigma\sqrt{\frac{k_B T}{\pi m}}$$

RESULTS AND DISCUSSION

Simulations are conducted for the model gas described in the preceding section, in the following conditions:

**Temperature:** $T = 285.71\ K$
Density: $n = 2.4 \cdot 10^{21}\ m^{-3}$

The fluctuation spectra are sampled at the wavelength $\frac{2\pi}{k} = 0.02\ m$. Since in the given conditions the mean free path is $\lambda_c = 4 \cdot 10^{-4}\ m$, the probed fluctuations fall into the hydrodynamic regime. Two situations are analyzed. In the first case, relaxation of internal energy is fast enough as compared to the flow characteristic time (as determined by the speed of sound). In these conditions we expect the one-temperature model to be accurate and that the two-temperature model reduce to the former. We choose: $p_0 = 0.1$ that gives for the relaxation time: $\tau \approx 7.0 \cdot 10^{-6}\ s$.

Figure 1 shows the fluctuation power spectra as obtained from DSMC simulations and from the one-temperature and two-temperature models, respectively. Also shown for comparison are the spectra predicted for the same gas when the internal energy relaxation is forbidden (frozen case) or when it is instantaneous (equilibrium case).

We see that, in this case, both models describe the DSMC results accurately. Comparison with the frozen and equilibrium cases also shows that this agreement is not trivial since there is an important contribution of the bulk viscosity to the spectrum:

$$\frac{\mu}{\eta} = 1.0$$

Note that the one-temperature model cannot describe the change in the speed of sound that is a consequence of the finite relaxation time for internal energy. For this case, however, the difference with respect to the equilibrium case is negligible.
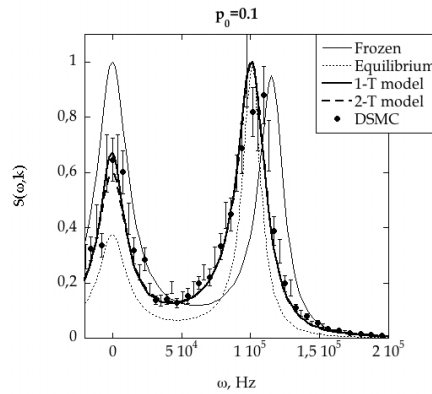
FIGURE 1. Fluctuation power spectra for the fast relaxation case.

As a second test with slow relaxation we choose: $p_0 = 0.01$, that gives for the relaxation time: $\tau \approx 7.0 \cdot 10^{-5}\ s$.

Figure 2 shows the fluctuation power spectra for this case. In this case, the one-temperature model fails to describe the transport properties of the system correctly. The two-temperature model, instead, gives an adequate description of the system behaviour and the agreement with the DSMC simulations is satisfactory.
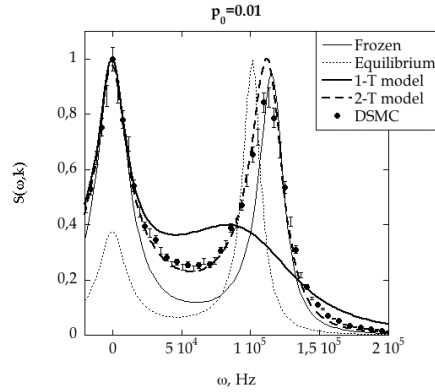
FIGURE 2.   Fluctuation power spectra for the slow relaxation case.

We conclude that multitemperature hydrodynamic equations, as derived from the Boltzmann transport equation, provide an adequate description of internal energy relaxation for all values of the relaxation time. Therefore there is no need to invoke frequency dependent transport coefficients that introduce unnecessary complications. Further, the results support the conclusion, obtained by kinetic theoretical arguments[5] that the multitemperature model reduces to the one-temperature model when the relaxation time is small enough and that only in this case a bulk viscosity formalism is adequate.

ACKNOWLEDGMENTS

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