Dissipative mass flux and sound wave propagation in monatomic gases

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Abstract. Predicting sound wave dispersion in monatomic gases is a fundamental gas flow problem in rarefied gas dynamics. The Navier-Stokes-Fourier model is known to fail where local thermodynamic equilibrium breaks down. Generally, conventional gas flow models involve equations for mass-density without a dissipative mass contribution. In this paper we observe that using a dissipative mass flux contribution as a non-local-equilibrium correction can improve agreement between the continuum equation prediction of sound wave dispersion and experimental data. Two mass dissipation models are investigated: a preliminary model that simply incorporates a diffusive density term in the set of three conservation equations, and another model derived from considering microscopic fluctuations in molecular spatial distributions.

Keywords: sound wave propagation; non-equilibrium gas dynamics; mass diffusion; gas kinetic theory; continuum fluid mechanics

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INTRODUCTION

A fundamental problem in gas kinetic theory is predicting the sound wave dispersion in monatomic gases. It is well-known that the Navier-Stokes-Fourier hydrodynamic model performs poorly on this problem in rarefaction regimes. From earlier investigations, various difficulties have also emerged when comparing theoretical results with experimental data; these include the correct formulations of the boundary value problem, utilization of appropriate boundary conditions, and definition of the time and length scales involved [1]. Three length (time) scales are involved in the sound wave dispersion analysis: the intermolecular mean free path, the propagating sound wavelength, and the separation distance between source and receiver. These three parameters lead to three different dimensionless quantities. Which of these three quantities are associated with the Knudsen number, depends on the researcher. Meanwhile, in the experimental protocol of Greenspan [2], varying the Knudsen number was accomplished by varying the distance between the source and receiver; whereas in the experiments by Schotter [3], the results are presented with that separation distance fixed and the propagating sound wave frequency varied. Among recent work, Garcia and Siewert provided numerical solutions using five kinetic models: the linearized Boltzmann equation, BGK model, S Model, Gross-Jackson model, MRS model, and CES model [4]. Their approach consisted of a half space bounded by a vibrating plate (the source) modeled as a perfectly diffuse reflection surface. They compared their results with experimental data by Schotter [3], and a discrepancy at high frequencies has been mentioned in their analysis [4]. This approach has been extended by Kalempa and Sharipov to incorporate also the boundary condition for the receptor [5].

It is clear that classical hydrodynamics, where flow variables are subject to a local thermodynamic equilibrium condition and macroscopic gradient effects are locally neglected, do not allow for a dissipative mass-density flux [6]. However, gas flows such as sound wave propagation in rarefied regimes are highly non-equilibrium. In this paper we show that using a dissipative mass flux contribution as a non-local-equilibrium correction, specifically in the evolution equation for the fluid mass-density, improves systematic agreement between the continuum model and experimental data. Two mass dissipation correction models are investigated. One is based on a simple dissipative correction to the mass-density equation within the set of three conservation equations, and the second is derived from considering microscopic fluctuations in molecular spatial distributions.
A SIMPLIFIED MASS DIFFUSION CONTINUUM MODEL

We consider a continuum model consisting of the classical conservation equations of mass, momentum and energy, but modified by a dissipative density flux:

**Mass-density**

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot [\rho U + J_m] = 0, \quad (1) \]

**Momentum**

\[ \frac{\partial \rho U}{\partial t} + \nabla \cdot [\rho U U] + \nabla \cdot [\rho I + \Pi] = 0, \quad (2) \]

**Energy**

\[ \frac{\partial}{\partial t} \left[ \frac{1}{2} \rho U^2 + \rho e_{in} \right] + \nabla \cdot \left[ \frac{1}{2} \rho U^2 U + \rho e_{in} U \right] + \nabla \cdot [(\rho I + \Pi) U] + \nabla \cdot [q] = 0, \quad (3) \]

where quantities \( J_m, \Pi, \) and \( q \), are all given a Fick’s law diffusive flux representation as:

\[ \Pi = -v \left[ \nabla (\rho U) + (\nabla (\rho U))^T \right] + \eta \nabla \cdot (\rho U) I, \]
\[ q = -\kappa_\text{h} \nabla (\rho e_{in}), \]
\[ J_m = -\kappa_m \nabla \rho. \]

In this set of equations, \( \rho \) denotes the fluid mass-density, \( U \) the flow unique velocity, and \( e_{in} \) the fluid local internal heat energy while \( I \) is the identity matrix. Furthermore, relation between temperature, \( T \), and internal energy are assumed given by \( e_{in} = 3/2RT \) with \( R \) being the specific gas constant, and Boyle’s Law holds for local flow properties, i.e., \( p = \rho RT \) with \( p \) denoting the pressure. Quantities \( J_m, \Pi, \) and \( q \) denote diffusive fluxes in addition to convective transport fluxes corresponding to mass, momentum, and energy respectively. These quantities are assumed resulting from existence of gradients and modeled here by Fick’s Law type of expression.

Compared with the traditional expression of the continuum set of conservation equations, a non-vanishing diffusive term, \( J_m \), introduced in the mass-density equation marks the only difference. Setting this term to zero as conventionally is consistent with neglecting, locally, gradients in mass-density field when expressing the local total mass flux. A non-vanishing \( J_m \) may find an interpretation where local gradients are no longer negligible or as a result of fluctuations in molecular spatial distributions [7]. Meanwhile, although one may expect the additional diffusive flux to affect momentum and energy equations within a methodical derivation of such a non-local-equilibrium continuum model, the above simplified model is adopted to identify implications of the single dissipative term in the mass-density equation for sound wave dispersion in gases. Diffusive fluxes in equations (4)-(6), are written such that primarily (constant) transport coefficients are the mass diffusivity coefficient \( \kappa_m \), the momentum density diffusivity coefficient \( \kappa_m \), that in turn define respectively a dynamic viscosity and a heat conductivity. Moreover, \( \eta \) is the bulk viscosity, so that \( \eta = 2/3v \) corresponds to Stokes’s assumption.

**Linearized one-dimensional equations**

For the sound wave propagation problem the set of equations (1) to (6) is considered in a one-dimensional configuration. An equilibrium ground state defined by the flow variables \( \rho^0, T^0, \rho^0 = R\rho^0 T^0, U_{m}^0 = 0 \), with \( R \) the specific gas constant. Then a perturbation from this ground state is introduced as follows:

\[ \rho = \rho^0(1 + \rho^*), \quad T = T^0(1 + \tau^*), \quad (7) \]
\[ U = U^*\sqrt{RT^0}, \quad p = p^0(1 + p^*), \]

where the asterisked variables represent dimensionless quantities. Linearizing \( p = \rho RT \) gives \( p^* = \rho^* + T^* \). The dimensionless space and time variables are given by,

\[ x = Lx^*, \quad t = \frac{L}{\sqrt{RT^0}}t^* = \tau t^*, \quad (8) \]
with $\tau = L/\sqrt{RT}$. Dimensionless linearized equations can therefore be written:

**Mass-density**

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial U^*}{\partial x^*} - \kappa_m \frac{\partial^2 \rho^*}{\partial x^2} = 0,$$

(9)

**Momentum**

$$\frac{\partial U^*}{\partial t^*} - \frac{4}{3} \nu \frac{\partial^2 U^*}{\partial x^2} + \frac{\partial \rho^*}{\partial x^*} + \frac{\partial T^*}{\partial x^*} = 0,$$

(10)

**Energy**

$$\frac{\partial T^*}{\partial t^*} + \frac{2}{3} \frac{\partial U^*}{\partial x^*} - \kappa_h \frac{\partial^2 T^*}{\partial x^2} + (\kappa_m - \kappa_h) \frac{\partial^2 \rho^*}{\partial x^2} = 0,$$

(11)

where the different dimensionless transport coefficients are given through:

$$\nu = L \sqrt{RT} \nu^*, \quad \kappa_m = L \sqrt{RT} \kappa_m^*, \quad \kappa_h = L \sqrt{RT} \kappa_h^*.$$  

(12)

Next we assume the disturbances $\rho^*, T^*$ and $U^*$ to be wave functions of the form:

$$\phi^* = \phi_u^* \exp[i(\omega t^* - K x^*)],$$  

(13)

where $\omega$ is the complex wave frequency, $K$ is the complex wave number, and $\phi_u^*$ is the complex amplitude, so that:

$$\frac{\partial \phi^*}{\partial t^*} = i\omega \phi^*, \quad \frac{\partial \phi^*}{\partial x^*} = -iK \phi^*, \quad \frac{\partial^2 \phi^*}{\partial x^2} = -K^2 \phi^*, \quad \frac{\partial^3 \phi^*}{\partial x^3} = iK^3 \phi^*.$$

The linearized hydrodynamic set of equations then yields the homogeneous system,

$$\begin{pmatrix}
  i\omega + \kappa_m^2 K^2 & 0 & -iK \\
  -K^2(\kappa_m^* - \kappa_h^*) & \kappa_h^* K^2 + i\omega & -\frac{2}{3}iK \\
  -iK & -iK & \frac{2}{3}v^* K^2 + i\omega
\end{pmatrix}
\begin{pmatrix}
  \rho^* \\
  T^*
\end{pmatrix} = 0.$$  

(14)

The corresponding dispersion relation from the degeneracy requirement is then:

$$K^2 (3\kappa_m K^2 - 4\mu (\omega - iK^2 \kappa_h)) + 5i\omega + \kappa_h (K^2 (3i\omega \kappa_h + 2) - 6\omega^2)) - 3i\omega^3 = 0,$$

(15)

which can be solved analytically when the three dimensionless transport coefficients are given by $\nu^* = \kappa_m^* = \kappa_h^* = 1$. This choice, together with Stokes’s assumption for the bulk viscosity $\eta$, is the one giving the best agreement with the experimental data presented in this paper.

**Definitions of dimensionless parameters**

The experimental set-up generated plane waves from a transmitter (the source), with a fixed experimental frequency, which then travelled through a gas and were recorded by a receiver [3, 8]. The receiver position and the pressure are primary control parameters to vary the rarefaction of the gas confined between source and receiver. Standing harmonic waves are observed during the experiments [3] that suggest that plane harmonic waves of the form of equation (13) are a suitable choice from the theoretical point of view. The various characteristic length scales involved in this configuration can therefore be listed as:

- the mean free path, $\lambda$, as the distance between two consecutive gaseous molecular collisions;
- the separation distance between the source and receiver, $L$;
- the experimental source sound wave length, $\lambda_s$ (or frequency $\omega_s$);
- the frequency of molecular collisions with boundaries, $f_w$ (or equivalent in distance, $\lambda_m$);
the average distance between molecules.

From the above list, we may generate the following list of dimensionless parameters.

\[ K_{n1} = \frac{\lambda}{\lambda_c}, \quad K_{n2} = \frac{\lambda_e}{\lambda_c}, \quad K_{n3} = \frac{\lambda_w}{\lambda_e} = \frac{C_0}{f_w L}. \]  

Expression \( K_{n2} \), which was the Knudsen number in [9], is now called the frequency ratio by more recent authors, such as [5], whereas the Knudsen number became instead \( K_{n1} \). The form of \( K_{n3} \) was inferred in [3].

In fact, starting from a harmonic plane wave of the form given in equation (13), one can show that, for high pressure and large source-receiver distances, the Knudsen number \( K_n \), the dimensionless sound wave speed \( \Upsilon \), and the damping coefficient \( \Lambda \) can be written (see appendix of [10]):

\[ K_n = \frac{\lambda}{\lambda_e} \Rightarrow \frac{1}{\Upsilon} = \sqrt{\frac{5}{3}} \text{Re}[K], \quad \Lambda = -\sqrt{\frac{5}{3}} \text{Im}[K]. \]  

In equations (17), the Knudsen number appears as a dimensionless wave number (or wave frequency) and the damping coefficient is a function of the wave frequency. Conversely, in equations (18), the Knudsen number now involves the source-receiver distance, and damping no longer depends on the wave frequency. These two sets of definitions better encompass the dominant effects of collisions between molecules at high pressure and large source-receiver separation distances, where boundary effects are negligible, and the dominant effects of collisions between molecules and surfaces for low pressure and small source-receiver separation distances.

**Dispersion and damping compared with experiments**

We first compare the sound wave speed and damping predicted by the diffusive mass-density modified dispersion relation, equation (15) with Navier-Stokes-Fourier (\( \kappa_m = 0 \)) results, using the hydrodynamic regime definition of the Knudsen number in equation (17) (so as in Greenspan [8]). Figures 1 and 2 show, respectively, the inverse phase speed and damping coefficient varying with inverse Knudsen number, with argon gas experimental data from [11]. It is clear that the diffusive mass-density term introduces an improvement in the Navier-Stokes-Fourier results. The previously large discrepancy between experimental and theoretical results is much smaller in the modified model. Broadly, both damping and speed agree with experiments well into the transition regime, up to \( Kn \approx 3 \). The Navier-Stokes-Fourier model fails at \( K_n \approx 0.2 \) on damping.
A VOLUME KINETIC MODEL FOR DISSIPATIVE MASS CONTRIBUTIONS

A volume kinetic approach was introduced in [7] where the concept of mass-density, defined as some amount of mass divided by a certain quantifiable volume, is given a different molecular level representation. This resulted in a set of continuum fluid equations where continuity equation was an expression of probability conservation and is separated from an evolution equation of the fluid mass-density. That mass-density evolution equation encompasses fluctuations in molecular spatial distribution, and involves a dissipative mass-density and a certain volume production term. In a one dimensional configuration, the dimensionless form of this model is given by [10]:

Continuity
\[
\frac{\partial A_n^*}{\partial t^*} + \frac{\partial U^*}{\partial x^*} = 0, \tag{19}
\]

Mass-density
\[
(1 - \chi^*) \frac{\partial p^*}{\partial t^*} - \kappa_m^* \frac{\partial^2 p^*}{\partial x^*^2} + (\alpha^* - \chi^*) \frac{\partial T^*}{\partial t^*} - \gamma^* \frac{\partial^2 T^*}{\partial t^*^2} + (\beta^* - \gamma^*) \frac{\partial^2 T^*}{\partial t^*^2} = 0, \tag{20}
\]

Momentum
\[
\frac{\partial U^*}{\partial t^*} - \frac{4}{3} \mu^* \frac{\partial^2 U^*}{\partial x^*^2} + \frac{\partial A_n^*}{\partial x^*} + \frac{\partial T^*}{\partial x^*} - \frac{4}{3} \mu^* \kappa_m^* \frac{\partial^3 p^*}{\partial x^*^3} = 0, \tag{21}
\]

Energy
\[
\frac{\partial T^*}{\partial t^*} + \frac{2}{3} \frac{\partial U^*}{\partial x^*} + \frac{2}{3} \kappa_m^* \frac{\partial^2 T^*}{\partial x^*^2} + \frac{5}{3} \kappa_m^* \frac{\partial^3 p^*}{\partial x^*^3} = 0. \tag{22}
\]

In these equations, \(A_n\) describes the probability of the presence of a gaseous molecule in a certain spatial region. Coefficients \(\alpha\) and \(\beta\) are first and second gas thermal expansion coefficients, while \(\chi\) and \(\gamma\) are first and second compressibility coefficients. These coefficients are involved in the description of the volume production term within the mass-density equation. Dynamic viscosity is denoted \(\mu\), and other variables have their meaning as defined in previous sections above.

Using a monatomic gas Prandtl number, and some combinations of the various expansion and compressibility coefficients, the wave speed predicted by equations (19) to (22) fits, in all regimes, the argon gas experimental data from [11] (see figure 3). Regarding the damping coefficient: with the hydrodynamic regime definition of the Knudsen number, agreement with experimental data is obtained up to a Knudsen number of about 1; conversely, using the rarefaction regime definition, good agreement is obtained at high Knudsen numbers (seen in figure 4).

CONCLUSION

Although conventional continuum models of gas flow do not include a dissipative mass flux, it has been shown in this paper that a dissipative mass flux can improve agreement in predicting sound wave dispersion in rarefaction regimes.
A methodical derivation of a full set of dissipative mass model with an assessment of its ability to predict known non-equilibrium flows are still very open questions however. The authors’s-volume based kinetic approach to deriving one of such models indicates that a dissipative term in the density equation is accompanied by a non-local-equilibrium form of the local total energy (energy functional) [7]. Meanwhile, modern non-equilibrium thermodynamic derivations show strong link between the adopted energy functional and its associated hydrodynamic models [12]. A local-equilibrium energy functional in which gradients are neglected is the essence of conventional continuum models leading to vanishing dissipative mass flux. But, an energy functional can also adopt a more general expression incorporating local gradient effects. By starting with this type of generalized functional energy it may be possible to obtain a full and thermodynamically consistent dissipative mass model. This will be considered in future work.

REFERENCES