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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. Attempts to solve this problem are therefore usually based on the Boltzmann equation. 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 predictions of sound wave dispersion when compared with 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

PACS: 43.35.-d,47.35.-i,42.25.Dd,47.10.-g,47.45.-n,47.70.Nd

INTRODUCTION

A fundamental problem in gas kinetic theory is predicting the sound wave dispersion in monatomic gases. It is now well accepted that the Navier-Stokes-Fourier hydrodynamic model performs poorly on this problem in rarefaction regimes. Most attempts to solve this problem have therefore been based on the Boltzmann kinetic equation and have not always been successful [1, 2]. From earlier investigations, various common difficulties have emerged: fitting experimental data over the full range of flow regime, correct formulations of the boundary value problem, utilization of appropriate boundary conditions, and definition of the time and length scales involved [1]. Concerning this last difficulty, 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 [2]. In the experimental protocol of Greenspan [3], varying the Knudsen number was accomplished by varying the distance between the source and receiver; whereas in the experiments by Schotter [4], 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 [5]. 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 [4], and a discrepancy at high frequencies has been mentioned in their analysis [5]. While neither traditional fluid models nor the Boltzmann ordinary kinetic equation include dissipative mass, it is shown in this paper that a dissipative mass flux improves systematically the agreement between the continuum model and experimental data for sound wave propagation.

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

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

Momentum

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

Energy

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

where quantities \mathbf{J}_m , Π , and \mathbf{q} , are all given a Fick's law diffusive flux representation as:

$$\Pi = -\nu [\nabla(\rho U) + (\nabla(\rho U))^tr] + \eta \nabla \cdot (\rho U) \mathbf{I}, \quad (4)$$

$$\mathbf{q} = -\kappa_h \nabla(\rho e_{in}), \quad (5)$$

$$\mathbf{J}_m = -\kappa_m \nabla \rho. \quad (6)$$

In this set of equations, ρ denotes the fluid mass-density, U the flow unique velocity, and e_{in} the fluid local internal heat energy while \mathbf{I} is the identity matrix. Furthermore, the relation between temperature, T , and internal energy is assumed to be 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 \mathbf{J}_m , Π and \mathbf{q} denote diffusive fluxes in addition to convective transport fluxes corresponding to mass, momentum, and energy respectively. These quantities are assumed to result from the existence of gradients and are modeled here by a Fick's Law type of expression.

Compared with the traditional expression of the continuum set of conservation equations, a non-vanishing diffusive term, \mathbf{J}_m , introduced in the mass-density equation marks the only difference. Setting this term to zero is consistent with neglecting, locally, gradients in the mass-density field when expressing the local total mass flux. A non-vanishing \mathbf{J}_m may find an interpretation where local gradients are no longer negligible, or as a result of fluctuations in molecular spatial distributions [6]. Although one may expect the additional diffusive flux to affect the 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 the (constant) transport coefficients are the mass diffusivity coefficient κ_m , the momentum density diffusivity coefficient (or kinematic viscosity) ν , the energy density diffusivity coefficient κ_h , that in turn define respectively a dynamic viscosity and a heat conductivity. Moreover, η is the bulk viscosity, so that $\eta = 2/3\nu$ 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 ρ^0 , T^0 , $p^0 = R\rho^0 T^0$, $U_m^0 = 0$, with R the specific gas constant. Then a perturbation from this ground state is introduced as follows:

$$\begin{aligned} \rho &= \rho^0(1 + \rho^*), & T &= T^0(1 + T^*), \\ U &= U^* \sqrt{RT^0}, & p &= p^0(1 + p^*), \end{aligned} \quad (7)$$

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 $\tau = L/\sqrt{RT^0}$. Dimensionless linearized equations can therefore be written:

Mass-density

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial U^*}{\partial x^*} - \kappa_m^* \frac{\partial^2 \rho^*}{\partial x^{*2}} = 0, \quad (9)$$

Momentum

$$\frac{\partial U^*}{\partial t^*} - \frac{4}{3}v^* \frac{\partial^2 U^*}{\partial x^{*2}} + \frac{\partial \rho^*}{\partial x^*} + \frac{\partial T^*}{\partial x^*} = 0, \quad (10)$$

Energy

$$\frac{\partial T^*}{\partial t^*} + \frac{2}{3} \frac{\partial U^*}{\partial x^*} - \kappa_h^* \frac{\partial^2 T^*}{\partial x^{*2}} + (\kappa_m^* - \kappa_h^*) \frac{\partial^2 \rho^*}{\partial x^{*2}} = 0, \quad (11)$$

where the different dimensionless transport coefficients are given through:

$$v = L\sqrt{RT^0}v^*, \quad \kappa_m = L\sqrt{RT^0}\kappa_m^*, \quad \kappa_h = L\sqrt{RT^0}\kappa_h^*. \quad (12)$$

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

$$\phi^* = \phi_a^* \exp[i(\omega t^* - Kx^*)], \quad (13)$$

where ω is the complex wave frequency, K is the complex wave number, and ϕ_a^* 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,

$$\begin{pmatrix} i\omega + \kappa_m^* K^2 & 0 & -iK \\ -K^2(\kappa_m^* - \kappa_h^*) & \kappa_h^* K^2 + i\omega & -\frac{2}{3}iK \\ -iK & -iK & \frac{4}{3}v^* K^2 + i\omega \end{pmatrix} \begin{pmatrix} \rho^* \\ T^* \\ U^* \end{pmatrix} = 0. \quad (14)$$

The corresponding dispersion relation from the degeneracy requirement is then:

$$\hat{k}^2 (3\hat{\kappa}_m \hat{k}^2 - 4\hat{\mu} (\omega - i\hat{k}^2 \hat{\kappa}_h)^2 + 5i\omega + \hat{\kappa}_h (\hat{k}^2 (3i\omega \hat{\kappa}_h + 2) - 6\omega^2)) - 3i\omega^3 = 0, \quad (15)$$

which can be solved analytically when the three dimensionless transport coefficients are given by $v^* = \kappa_m^* = \kappa_h^* = 1$. This choice, together with Stokes's assumption for the bulk viscosity η , 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 frequency, which then travelled through a gas and were recorded by a receiver [4, 7]. The receiver position and the pressure are the primary control parameters to vary the rarefaction of the gas confined between source and receiver. Standing harmonic waves are observed during the experiments [4] 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, λ , as the distance between two consecutive gaseous molecular collisions;
- the separation distance between the source and receiver, L ;
- the experimental source sound wave length, λ_e (or alternatively the frequency ω_e);
- the frequency of molecular collisions with boundaries, f_w (or alternatively the distance λ_w);
- the average distance between molecules.

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

$$K_{n1} = \frac{\lambda}{L}, \quad K_{n2} = \frac{\lambda}{\lambda_e}, \quad K_{n3} = \frac{\lambda_w}{L} = \frac{C_0}{f_w L}. \quad (16)$$

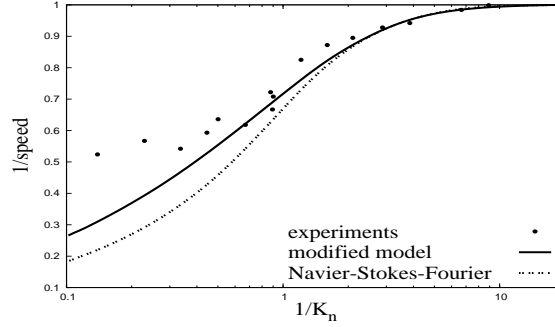


FIGURE 1. Normalized inverse phase speed varying with inverse Knudsen number, as predicted by equation (15).

In various references dealing with sound wave propagation in monatomic gases and comparing these with the experiments, the dimensionless parameters in expressions (16) have been treated as Knudsen numbers differently. Expression K_{n2} , which was the Knudsen number in [8], is now called the frequency ratio by more recent researchers whereas the Knudsen number became instead K_{n1} . The form of K_{n3} was inferred in [4].

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 Υ , and the damping coefficient Λ can be written (see appendix of [9]):

$$K_n = \frac{\lambda}{\lambda_e} \Rightarrow \frac{1}{\Upsilon} = \sqrt{\frac{5}{3}} \frac{Re[K]}{\omega}, \quad \Lambda = -\sqrt{\frac{5}{3}} \frac{Im[K]}{\omega}. \quad (17)$$

These definitions are valid in the hydrodynamic regime, and correspond to the dimensionless analysis first introduced by Greenspan to examine his experimental data. In contrast, for low pressure and small source-receiver separation distances, the definitions in equation (17) change to,

$$K_n = \frac{\lambda_w}{L} \Rightarrow \frac{1}{\Upsilon} = \sqrt{\frac{5}{3}} \frac{Re[K^*]}{\omega^*}, \quad \Lambda = -\sqrt{\frac{5}{3}} \frac{Im[K^*]}{\omega^*}. \quad (18)$$

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 at 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 the Navier-Stokes-Fourier ($\kappa_n = 0$) model, using the hydrodynamic regime definition of the Knudsen number in equation (17) (so as in Greenspan [7]). Figures 1 and 2 show, respectively, the inverse phase speed and damping coefficient varying with inverse Knudsen number, with argon gas experimental data from [10]. 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 pure Navier-Stokes-Fourier model fails at $Kn \approx 0.2$ on damping.

A VOLUME KINETIC MODEL FOR DISSIPATIVE MASS CONTRIBUTIONS

A volume kinetic approach was introduced in [6] 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

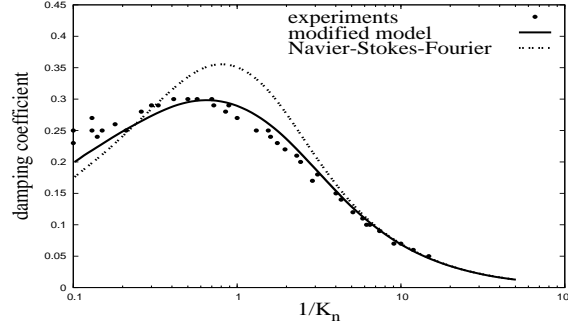


FIGURE 2. Normalized damping coefficient varying with inverse Knudsen number, as predicted by equation (15).

set of continuum fluid equations where the 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 [9]:

Continuity

$$\frac{\partial A_n^*}{\partial t^*} + \frac{\partial U^*}{\partial x^*} = 0, \quad (19)$$

Mass-density

$$(1 - \chi^*) \frac{\partial \rho^*}{\partial t^*} - \kappa_m^* \frac{\partial^2 \rho^*}{\partial x^{*2}} + (\alpha^* - \chi^*) \frac{\partial T^*}{\partial t^*} - \gamma^* \frac{\partial^2 \rho^*}{\partial t^{*2}} + (\beta^* - \gamma^*) \frac{\partial^2 T^*}{\partial t^{*2}} = 0, \quad (20)$$

Momentum

$$\frac{\partial U^*}{\partial t^*} - \frac{4}{3} \mu^* \frac{\partial^2 U^*}{\partial x^{*2}} + \frac{\partial A_n^*}{\partial x^*} + \frac{\partial T^*}{\partial x^*} - \frac{4}{3} \mu^* \kappa_m^* \frac{\partial^3 \rho^*}{\partial x^{*3}} = 0, \quad (21)$$

Energy

$$\frac{\partial T^*}{\partial t^*} + \frac{2}{3} \frac{\partial U^*}{\partial x^*} - \frac{2}{3} \kappa_h^* \frac{\partial^2 T^*}{\partial x^{*2}} + \frac{5}{3} \kappa_m^* \frac{\partial^2 \rho^*}{\partial x^{*2}} = 0. \quad (22)$$

In these equations, A_n describes the probability of the presence of a gaseous molecule in a certain spatial region. Coefficients α and β are first and second gas thermal expansion coefficients, while χ and γ 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 μ , and other variables have their meaning as defined in the 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 [10] (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 higher Knudsen numbers (seen in figure 4).

CONCLUSION

Dissipative mass/density in classical hydrodynamics, with total energy and entropy given local-equilibrium expressions and the Gibbs relation, have been considered in [11] and the authors have shown that they are incompatible; particularly with respect to some properties, such as angular momentum conservation. However, a dissipative mass flux reflects non-local equilibrium behaviour that the local-equilibrium foundations of classical hydrodynamics consider to be negligible when defining local thermodynamic variables. It is known that in strong disequilibrium, local

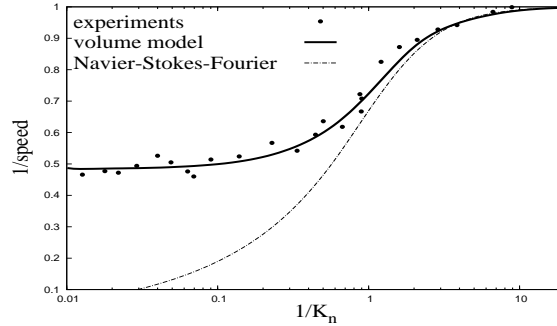


FIGURE 3. Normalized inverse phase speed varying with inverse Knudsen number, as predicted by the volume kinetic model for dissipative mass contributions

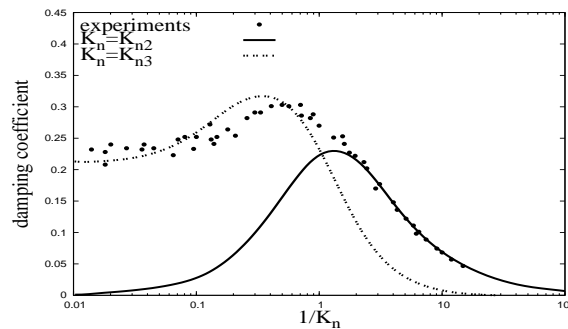


FIGURE 4. Normalized damping coefficient varying with inverse Knudsen number, as predicted by the volume kinetic model for dissipative mass contributions

total energy and entropy may have different expressions involving gradients [12]. Moreover, the local ‘volume’ containing the material under investigation is usually not mentioned as a variable when one derives local momentum conservation in the classical sense of Newton’s Laws of dynamics. Derivation of a dissipative mass model for fluids, as well as assessing its thermodynamic consistency, are therefore still very open questions. In any case, as experimental evidence is more credible than theoretical arguments, this article has been concerned with evaluating the effect of including a mass-diffusion term on an unsolved problem of sound wave propagation in rarefied gases; here we have shown it to have positive impact. Future work will include investigating the ability of the mass-diffusion component to handle other problematic rarefied flow configurations.

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