



INVESTIGATION OF AMPLITUDE DEPENDENCE ON NONLINEAR ACOUSTICS USING THE DIRECT SIMULATION MONTE CARLO METHOD

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Hanford, Amanda D.¹; Long, Lyle N.²

¹The Pennsylvania State University; University Park, PA, 16803, United States of America;
ald227@psu.edu

²The Pennsylvania State University; University Park, PA, 16803, United States of America;
lnl@psu.edu

ABSTRACT

Traditionally, acoustics is concerned with the treatment of the fluid as a continuum using macroscopic quantities such as velocity and pressure as dependent variables. However, the continuum model breaks down for Knudsen numbers (Kn) greater than roughly 0.05, where Kn is defined as the ratio of mean free path to wavelength. Particle methods are necessary for, but not limited to, problems with $Kn > 0.05$. The Knudsen number is large for sound propagation in very dilute gases, or at high frequencies and thus requires a particle method (or Boltzmann equation) solution. In our studies we have used a particle method, the direct simulation Monte Carlo (DSMC) method, for the direct physical modeling of particle motions and intermolecular collisions in nonlinear acoustics problems. Using DSMC to study nonlinear acoustics allows us to explore real gas effects for all values of Kn with a molecular model that continuum methods cannot offer. DSMC results for the absorption of sound have shown that absorption depends heavily on Kn and amplitude and deviates significantly from the continuum classical assumption for large Kn . In our current DSMC calculations we have explored the relationship between absorption and nonlinearity as a function of amplitude for a range of Knudsen numbers.

INTRODUCTION

There is a hierarchy of mathematical models available to solve fluid dynamics problems. These models have varying degrees of approximation but can be categorized into two groups: continuum and non-continuum methods. Continuum methods, which are popular for acoustic problems, model the fluid as a continuous medium. This model describes the state of the fluid with macroscopic level using quantities such as density, velocity, and temperature. The continuum approximation is valid when the characteristic length of the problem is much larger than the molecular spacing between fluid particles. This assumption is satisfied for many engineering problems, and thus fluid evolution can be described using continuum equations such as the Navier-Stokes, Euler or wave equations.

However, the continuum model has its limitations. The macroscopic model assumes deviations from thermal equilibrium are small, and it is the failure of the closure of the Navier-Stokes equations that limit the applications of this approach. The Knudsen number (Kn) which is defined to be the mean free path divided by a characteristic length scale is a measure of the nonequilibrium or viscous effects of the gas. The Knudsen number is also used to distinguish the regimes where different governing equations of fluid dynamics are applicable. The Navier-Stokes equations are valid for $Kn < 0.05$, and the Navier-Stokes equations reduce to the Euler equations as Kn approaches 0. The Boltzmann equation is the mathematical model for non-continuum methods and is valid for all Kn , although most efficient for high Kn . Therefore, non-continuum (or particle methods) are necessary for, but not limited to, problems where the Knudsen number is greater than 0.05.

Non-continuum methods are based on molecular models that realize the particle nature of the gas and describe the state of the gas at the microscopic level. Despite the fact that the Boltzmann equation was derived using a microscopic approach, it can be shown that the

Boltzmann equation will reduce to the continuum conservation equations (e.g Navier-Stokes) for low Kn [1].

Direct simulation Monte Carlo (DSMC) is a stochastic, particle-based method developed by Bird [1] that is capable of simulating real gas effects for all values of Kn with a molecular model that traditional continuum models cannot offer. The Knudsen number is large for sound propagation in very dilute gases or at high frequencies requiring a particle-method solution. Past results in DSMC showed that sound absorption depends heavily on Kn for acoustic wave propagation in monatomic gases [2]. Successful application of DSMC to nonlinear acoustic waves has already been shown for monatomic and diatomic gases [2, 3]. We continue to investigate this topic with the study of absorption with a more in depth emphasis on amplitude dependence and nonlinearity at high Kn. DSMC simulation results are examined at a variety of amplitudes and Knudsen numbers in gaseous argon to gain a broader understanding of the effects of amplitude and nonequilibrium for nonlinear acoustics applications.

For high amplitude sound propagation at atmospheric conditions, continuum equations such as the nonlinear Euler and Navier-Stokes equations have been widely used to understand the physical properties of sound due to nonlinearity. However, an overview of such approaches reveals that nonlinear effects are often treated separately, and then superimposed to produce a final result [4]. Instead of employing this technique, a method such as DSMC can model all nonlinear and viscous effects in the same method.

DIRECT SIMULATION MONTE CARLO

Direct simulation Monte Carlo was first introduced in 1963 by G. A. Bird [1] and has become a very versatile simulation tool. DSMC was originally developed for use in the aerospace engineering field for re-entry problems or rocket plume modeling, has been successfully used in various systems including but not limited to: hypersonic flows [5], rarefied gas dynamics [1], chemical reactions and detonations [6], and acoustics [2,3,7] including the study of the acoustic environment in planetary environments [8]. DSMC describes the dynamics of a gas through direct physical modeling of particle motions and collisions. DSMC is based on the kinetic theory of gas dynamics, where representative particles are followed as they move and collide with other particles. The movement of particles is determined by their velocities, while the collisions are determined statistically, but are required to satisfy mass, momentum, and energy conservation. In DSMC the particle positions and velocities are initialized randomly and the boundary conditions ultimately determine the final solution.

THEORY

The classical linear theory of sound propagation assumes that all acoustic fields can be written as the sum of an equilibrium value ψ_0 and a harmonic plane wave in the x direction which can be written in general form as:

$$\psi = \psi_0 + \psi' \exp[i(\omega t - kx)] \quad (\text{Eq. 1})$$

where ψ' is the acoustic amplitude, which is considered to be small, ω is the frequency in rad/s, k is the propagation constant, and t is time [9]. Substitution of the expression given by Eq [1] into thermodynamic equations, such as the Navier-Stokes equations, one can derive a dispersion relation from the continuity of momentum, mass and energy equations, written in terms of the complex valued propagation constant $k = \alpha + i\beta$, where α is the classical absorption coefficient and $\beta = c/c_0$ is the scaled phase speed for translational relaxation. This dispersion relation is given by the equation [10]:

$$\left(\frac{\omega}{c_0}\right)^2 + \left[1 + i\frac{\omega}{c_0^2}\left(\frac{4}{3}\frac{\mu}{\rho_0} + \frac{\kappa}{\rho_0 c_v}\right)\right]k^2 + \frac{\kappa}{\omega\rho_0 c_v}\left(\frac{i}{\gamma} - \frac{4}{3}\frac{\omega\mu}{c_0^2\rho_0}\right)k^4 = 0 \quad (\text{Eq. 2})$$

where c_0 is the low frequency, low amplitude speed of sound, ρ_0 is the ambient density, γ is the ratio of specific heats, μ is the coefficient of viscosity, κ is the coefficient of thermal conductivity, and c_v is the specific heat at constant volume.

In the limit of low frequencies, α becomes the familiar expression:

$$\alpha = \frac{\omega^2}{2\rho_0 c^3} \left(\frac{4}{3}\mu + \frac{(\gamma-1)\kappa}{\chi_v} \right) \quad (\text{Eq. 3})$$

and the phase speed becomes the adiabatic sound speed given by:

$$c = \sqrt{\gamma \frac{R}{M} T_0} \quad (\text{Eq. 4})$$

where R is the universal gas constant, M is molecular weight and T_0 is the equilibrium temperature [9].

Furthermore, this theory predicts that not only does the amplitude ψ' decay exponentially as a function of distance x , but that the propagation constant, k , is independent of the distance x from the source. These results are only valid for low amplitude sound where $\psi' \ll \psi_0$ and for low frequency where Kn is small (i.e. < 0.05). Comparison between the above classical predictions for the absorption of low amplitude sound and experiment show poor agreement at high Kn due to the invalid continuum assumption at high Kn [11, 12]. In addition, the collision of particles with the receiver introduces the propagation constant x dependence, and is also dependent on receiver size [13]. Several molecular-kinetics adjustments have been made to the theory to account for the discrepancy at high Kn with varying degrees of success. Sutherland and Bass [14] use an empirical adjustment to account for the high Kn behavior while Buckner and Ferziger [15] and Sirovich and Thurber [16] use approximations to the Boltzmann equation to describe deviation from the Navier-Stokes prediction for a monatomic gas. However, not all these presentations took into account the dependence of the propagation constant on x and no work has been done to investigate on the dependence of amplitude. Therefore, large discrepancies between experiment and theory still exist.

SIMULATION APPROACH

Since absorption mechanisms are inherently molecular properties, it is a natural progression to use a particle method for analysis. Because of the uncertainty of the relative importance of relaxation effects and nonlinearity on the absorption of sound at high Kn , we were interested in investigating the dependence of amplitude.

Acoustic waves were generated in the simulation domain by creating a piston boundary condition at one end of the domain. The velocity amplitude of the piston source ranged from 5 m/s to 45 m/s. Results for varying Kn were simulated in gaseous argon as hard sphere molecules at 273 K (molecular weight $M = 39.94$ and hard sphere diameter $\sigma = 3.66 \times 10^{-10}$ m). The variation in Kn was obtained by maintaining the cells per wavelength constant at 100, but varying the cell size from 1/2 of a mean free path to 1/200 of a mean free path. Each cell contained 150 particles per cell on average.

The time step was taken to be at least an order of magnitude smaller than the mean collision time and is on the order of picoseconds for each case. Care was taken that the time step remained smaller than the acoustic period of oscillation. Each case was initialized to start in thermal equilibrium, however relaxation is a nonequilibrium process, most notable at high Kn .

In order to take into account the dependence on distance, the parameter $\omega x / c_m = 10$ [12] is used as a nondimensional distance where c_m is the mean molecular velocity of the gas.

A parallel, object-oriented DSMC solver was developed for this problem. The code was written in C++ and Message Passing Interface (MPI) for interprocessor communication, and was run on massively parallel computers. The object-oriented approach allows the DSMC algorithm to be divided into physical objects that are individually maintained. Cell and Particle classes were created to govern fundamental components of the algorithm. With this object oriented technique it was possible to develop a C++ code that was easy to read, maintain and modify.

Despite excellent parallel efficiency, CPU time and memory requirements were quite large, taking approximately 6 hours on 32 processors for each run. Given the statistical nature of DSMC, there is an intrinsic degree of scatter in the simulation results.

RESULTS

The absorption sound as a function of amplitude

The scaled absorption α/k_0 as a function of Kn is shown in Figure 1, where $k_0 = \omega/c_0$ is the low frequency, low amplitude wave number. DSMC results are shown with the Navier-Stokes theoretical predictions and the low frequency approximation for the classical absorption coefficient given by Equations [2] and [3]. The results for the different piston amplitudes are shown for a range of Kn in each case. The scaled absorption data was computed at the scaled distance parameter $\omega x/c_m = 10$ for each case. Large deviations from continuum theory are seen for high Kn, as expected. The differences between the scaled absorption for different amplitudes are small at the distance of $\omega x/c_m = 10$ for high and low Kn. For Kn near the relaxation frequency, the amount of absorption depends heavily on the amplitude. Despite the small differences in the scaled absorption coefficient at low and high Kn, nonlinear effects are evident in the larger amplitudes as seen in Figure 2 with significant wave steepening for the Kn = 0.02, 45 m/s amplitude case, for example. The distance given by $\omega x/c_m = 10$ was calculated to be smaller than the traditional shock formation distance in each case given by the equation [4, 9]:

$$\bar{x} = \frac{\rho_0 c_0^2}{\beta k_0 P_0} \quad (\text{Eq. 5})$$

where β is the coefficient of nonlinearity, which is 4/3 for a monatomic gas, and P_0 is the acoustic pressure amplitude. However, this parameter is derived from the continuum approximation and is not necessarily valid for high Kn.

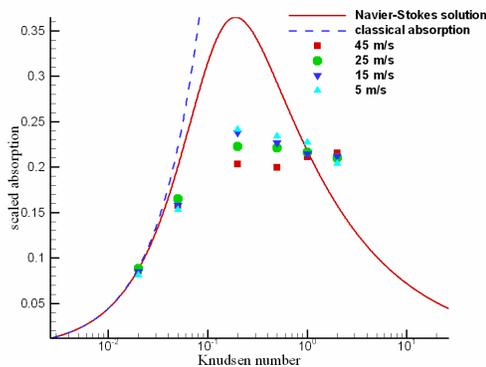


Figure 1.- absorption as a function of Kn for multiple amplitudes at $\omega x/c_m = 10$

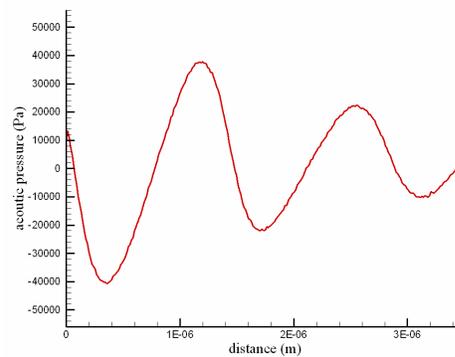


Figure 2.-wave steepening at Kn = 0.02.

When distances greater than $\omega x/c_m = 10$ are considered, nonequilibrium and nonlinear effects become more important in the evolution of sound propagation. The pressure amplitude as a function of distance for the Kn = 2, 5 m/s and 45 m/s cases are shown in Figures 3 and 4 respectively. For the high amplitude case in Figure 4, it is seen that the pressure amplitude from the DSMC simulation does not fit an exponential decay model, where as the lower amplitude case in Figure 3 does. It is believed that this behavior is a unique combination of nonlinear effects and nonequilibrium effects at high Kn. Figure 5 plots the translational nonequilibrium effects, T_x/T , for the Kn = 2, 45 m/s case at a snapshot in time. There is almost a 20% difference between T_x and T indicating strong nonequilibrium. Even at large amplitudes, nonequilibrium effects for lower Kn (Kn = 0.02, 45 m/s amplitude in this case),

which can not be determined by continuum approaches, are an order of magnitude smaller than for high Kn, as shown in Figure 6.

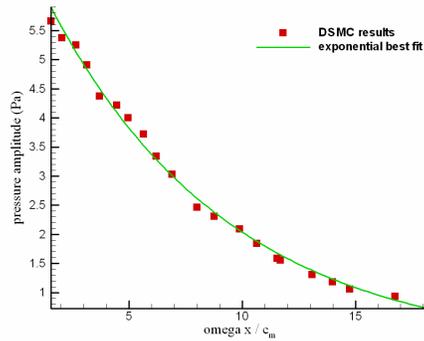


Figure 3.- amplitude as a function of distance for Kn = 2, 5 m/s

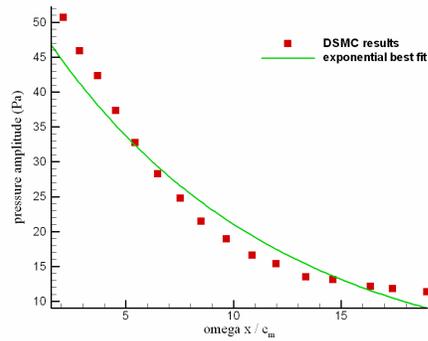


Figure 4.- amplitude as a function of distance for Kn = 2, 45 m/s

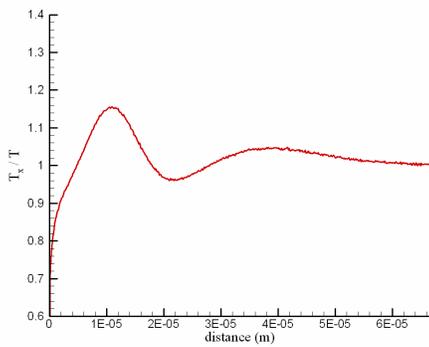


Figure 5 – nonequilibrium effects for Kn = 2

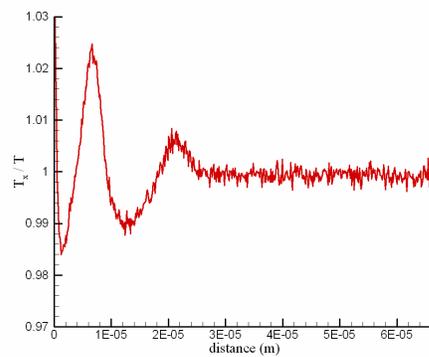


Figure 6. – nonequilibrium effects for Kn = 0.02

Nonlinear effects may also play a role in the nonexponential decay of high Kn, high amplitude sound. The normalized Fourier component amplitudes of the first 3 harmonics for Kn = 0.02 and Kn = 2 at 45 m/s amplitude are plotted against the nondimensional distance $\sigma = x / \bar{x}$ in Figures 7 and 8. The 2nd and 3rd harmonics are more dominant in the Kn = 2 case than in the Kn = 0.02 case, despite faster decay.

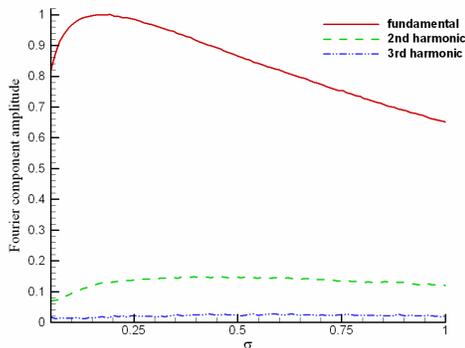


Figure 7 – Fourier component amplitudes for Kn = 0.02

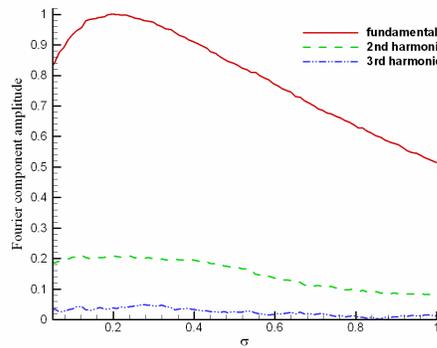


Figure 8. – Fourier component amplitudes for Kn = 2

CONCLUSIONS

Using the direct simulation Monte Carlo method, it is possible to simulate the details of nonlinear acoustic problems for a wide range of Knudsen numbers. An investigation on the amplitude dependence of the scaled absorption coefficient was performed for a wide range of Kn and amplitudes. Large deviations from continuum theory is seen for high Kn, but differences between amplitudes were small except for around the relaxation frequency at a nondimensional distance of $\omega x/c_m = 10$, despite nonlinear effects. For distances beyond $\omega x/c_m = 10$ nonlinear and nonequilibrium effects create nonexponential decay for high Kn, high amplitude sound. Nonequilibrium effects were evident in the simulations, even at low Kn.

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