

Molecular Relaxation Simulations in Nonlinear Acoustics using Direct Simulation Monte Carlo

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Abstract. The direct simulation Monte Carlo (DSMC) method describes gas dynamics 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. DSMC provides a useful tool for capturing all physical properties of interest for nonlinear acoustic problems, such as dispersion, attenuation, absorption, harmonic generation and nonequilibrium effects. The validity of DSMC for the entire range of Knudsen numbers (Kn), where Kn is defined as the mean free path divided by the wavelength, allows for the exploration of sound propagation at low Kn (low frequency, atmospheric conditions) as well as sound propagation at high Kn (high frequency, dilute gases, or in microdevices). For low Kn, nonlinear effects play an important role in waveform evolution. For high Kn, nonequilibrium effects are strong and increased absorption cancels out nonlinearity effects.

Keywords: DSMC, Monte Carlo, Absorption, Dispersion, Relaxation.

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INTRODUCTION

It is widely known that viscous, thermal and molecular relaxation losses play an important role in sound propagation in the atmosphere. Traditionally, acoustics is concerned with the treatment of the fluid as a continuum using macroscopic quantities such as density, velocity and pressure as dependent variables. However, the continuum model has its limitations and the model breaks down for Knudsen numbers (Kn) greater than 0.1, where Kn is defined as the mean free path divided by the wavelength. On the other hand, particle methods are necessary for, but not limited to, problems with $Kn > 0.1$. Since absorption mechanisms are inherently molecular properties, it is a natural progression to use a particle method for analysis.

Direct simulation Monte Carlo (DSMC) [1] is the particle method used in this study. DSMC is a stochastic method used to computationally model gas flows with thousands or millions of representative molecules through the direct physical modeling of particle motions and intermolecular collisions. Using DSMC to study acoustic waves allows us to explore real gas effects for all values of Kn with a molecular model that traditional continuum methods cannot offer.

The Knudsen number is large for sound propagation in very dilute gases or at high frequencies requiring a particle-method solution. DSMC results for acoustic wave

propagation in monatomic gases have shown that sound absorption depends heavily on Kn [2]. Successful application of the DSMC method to nonlinear acoustic waves has already been completed in monatomic and diatomic gases [2,3]. For this paper DSMC was used to study the interaction between acoustic absorption and nonlinearity through bimolecular collisions in mixtures of air containing water vapor for varying Kn.

DIRECT SIMULATION MONTE CARLO

Direct simulation Monte Carlo is a very versatile simulation tool, and has been successfully used in various systems including but not limited to: hypersonic flows, rarefied gas dynamics [1], chemical reactions [4], and acoustics [2,3]. The current model contains a phenomenological approach to simulate diatomic and polyatomic molecules in systems containing several species. This approach, developed by Larsen and Borgnakke [5], handles the internal energy exchange between the molecules during collisions. The theory assumes that a fraction of the collisions are regarded as inelastic, redistributing post-collision energy in a stochastic manner to produce physically realistic behavior at the macroscopic level. In this study, the molecules themselves will be considered in a classical sense as hard sphere molecules adhering to the Larsen-Borgnakke phenomenological approach.

SIMULATION APPROACH

Under standard atmospheric conditions, roughly 99% of dry air is composed of nitrogen, oxygen and trace amounts of carbon dioxide, argon, neon, methane, etc. The introduction of water vapor to a dry air mixture has been shown to be an important factor in absorption due to molecular relaxation [6,7]. The simulations generated in this research therefore focus entirely on nitrogen, oxygen and water vapor mixtures. The acoustic frequency of maximum absorption is called the relaxation frequency, and is a strong function of temperature.

Acoustic waves were generated in the simulation domain by creating a sinusoidal density distribution of specified frequency. In all cases, the acoustic density amplitude of the sinusoidal source is 20% of the ambient density, with an initial acoustic flow velocity equal to zero. Results for a single frequency at varying humidities were computed in a gas mixture, as well as a single humidity for varying Kn to investigate the results different absorption effects.

A parallel, object-oriented DSMC solver was developed for this problem. The code was written in C++ and was run on massively parallel computers. Despite excellent parallel efficiency, CPU time and memory requirements were quite large, taking approximately 60 hours on 32 processors for each run.

ABSORPTION AT LOW KN WITH VARYING HUMIDITY

Due to computational limitations and the strong dependence of the relaxation frequency to temperature, the DSMC simulations in a mixture of oxygen, nitrogen and water vapor were run at standard atmospheric pressure (ambient pressure = 101000

Pa) and a temperature of 373 K. The relaxation frequency at this temperature is approx 2 MHz, and is the frequency used in this study. The absorption coefficient for varying humidities is plotted with theory [6] in figure 1.

Due to the high amplitudes of the simulation at low Kn, we expect nonlinear effects to become important in the evolution of the sound wave. The shock formation distance at this frequency is beyond the simulation domain. However, considerable wave steepening was observed and is shown in figure 2.

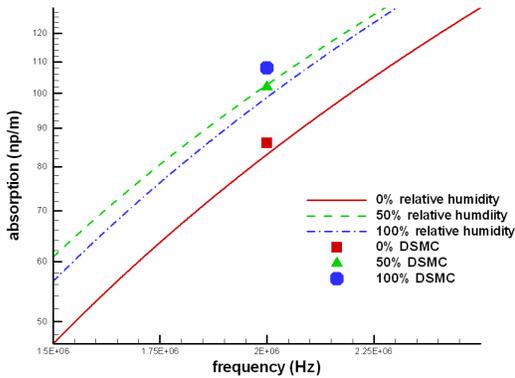


FIGURE 1. Absorption coefficient

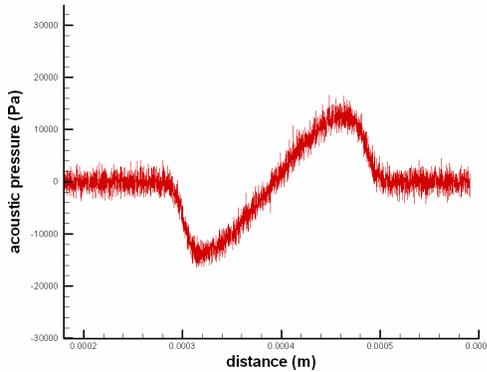


FIGURE 2. Wave steepening for 50% RH wave

ABSORPTION AT HIGH KN

The scaled absorption coefficient, α/k_0 where α is the absorption coefficient and k_0 is the acoustic wave number, for Kn ranging from 0.04 to 35 is shown in figure 3. DSMC simulation results are compared to a classical Navier-Stokes prediction, experimental work by Greenspan, and previous results for monatomic gas [2]. 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 3/1000 of a mean free path.

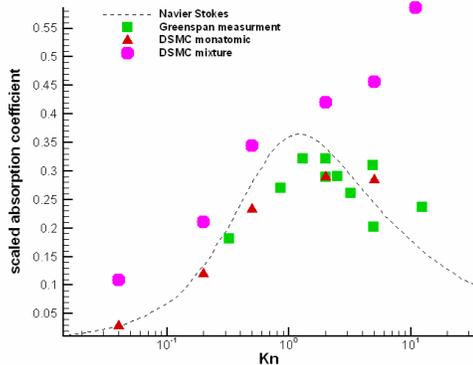


FIGURE 3. Scaled absorption vs. Kn

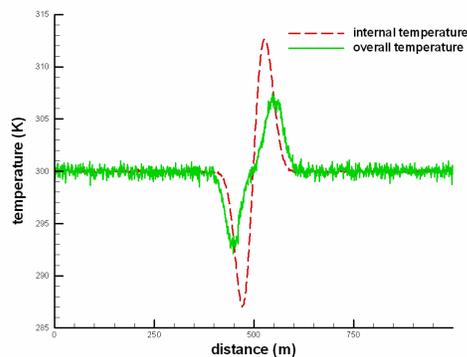


FIGURE 4. Nonequilibrium effects at Kn = 5

Figure 3 shows an increase in absorption due to molecular relaxation for gas mixtures compared to monatomic cases. When a gas is in thermal equilibrium the

internal, translational, and overall temperatures are equal. However, nonequilibrium effects become more important as Kn increases. The strong nonequilibrium effects are shown in figure 4, where internal and overall temperature are plotted with distance at a snapshot in time, as the acoustic wave propagates at $Kn = 5$. The time delay and magnitude difference between the two curves is evident, indicating molecular relaxation. These strong nonequilibrium effects play an important role in the increased absorption at high Kn .

Despite the fact that the acoustic density amplitude is 20% of the ambient density in these high Kn cases, the absorption is so great that nonlinear effects are very small. There is no evidence of wave steepening or shock wave formation.

CONCLUSIONS

Given the statistical nature of DSMC, there is an intrinsic degree of scatter in the simulation results. This universal drawback of DSMC makes it difficult in certain cases to produce adequate resolution, and is a source of limitation for this work.

The inclusion of internal energy in diatomic and polyatomic species has allowed us to investigate absorption and nonlinearity in gas mixtures. Increasing the relaxation collision number of a species affects the amount of nonequilibrium in the relaxation process. In this study it was determined that at low Kn there are nonequilibrium effects in mixtures with high concentrations of water, but the overall effect is small compared to the classical absorption coefficient. For mixtures with high Kn the nonequilibrium effects are very prominent and result in a much larger absorption coefficient.

Future work will include more detailed investigations into the internal energy configurations of diatomic and polyatomic molecules, the temperature dependence of relaxation collision numbers, and modeling characteristic temperatures of molecules

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