A low noise discrete velocity method for the Boltzmann equation with quantized rotational and vibrational energy

Peter Clarke *, Philip Varghese *, David Goldstein

ASE-EM Department, The University of Texas at Austin, 210 East 24th Street, Austin, TX 78712, USA

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A B S T R A C T

A discrete velocity method is developed for gas mixtures of diatomic molecules with both rotational and vibrational energy states. A full quantized model is described, and rotation–translation and vibration–translation energy exchanges are simulated using a Larsen–Borgnakke exchange model. Elastic and inelastic molecular interactions are modeled during every simulated collision to help produce smooth internal energy distributions. The method is verified by comparing simulations of homogeneous relaxation by our discrete velocity method to numerical solutions of the Jeans and Landau–Teller equations, and to direct simulation Monte Carlo. We compute the structure of a 1D shock using this method, and determine how the rotational energy distribution varies with spatial location in the shock and with position in velocity space.

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1. Introduction

The classical form of the Boltzmann equation is formulated for monatomic gases without internal structure and gas mixtures only. However, most gas flows of practical interest are made up of polyatomic molecules with rotational and vibrational energy. Wang Chang and Uhlenbeck [1] used quantized models of the internal energy levels and derived a form of the Boltzmann equation commonly referred to as the Wang Chang–Uhlenbeck equation, written as:

$$\frac{\partial \varphi_j}{\partial \tau} + \eta \frac{\partial \varphi_j}{\partial x} = I_j \tag{1}$$

where φ_j is the velocity distribution function for the jth internal energy level, η is a particular (vector) velocity, and τ and x represent time and space coordinates respectively. I_j is the collision operator for the jth internal energy level due to collisions with all other energy levels (k) resulting in transitions from levels (jk) to levels (lm). The collision operator is given in equation (2) below but a more convenient form for this work is presented in equation (9).

$$I_j = \sum_{klm} \int_{\hat{\zeta}} \left[\frac{q_l q_m}{q_j q_k} \varphi_l(\eta') \varphi_m(\zeta') - \varphi_j(\eta) \varphi_k(\zeta) \right] g \sigma_T (jk \to lm) dV_\zeta \tag{2}$$

The direct simulation Monte Carlo (DSMC) method has commonly been used to simulate low density nonequilibrium flows of gases with internal energy [2]. However, the simulation of nonequilibrium internal energy distributions can be

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* Corresponding authors.
E-mail addresses: peter.clarke29@gmail.com (P. Clarke), varghese@mail.utexas.edu (P. Varghese).

difficult for traditional particle methods such as DSMC if internal energy levels with very small fractional populations are important. In order to resolve these levels with any precision, a large number of particles and/or a large number of ensemble averages are needed. This can be computationally expensive. Discrete velocity methods for the Boltzmann equation may be used to address these inefficiencies since such models can have relatively little inherent noise and they can simulate large variations in densities efficiently.

For instance, the discrete velocity method can provide the structure of internal energy distributions at various locations within a shock without additional computational effort. Such investigations may be important when simulating processes such as non-equilibrium chemical reactions that are dependent on the internal energy distribution. The propagation of a combustion or detonation wave through a gas may depend on differences in the internal energy distributions of low and high speed particles. Similarly, the computation of the structure of dissociating and ionizing shocks requires the accurate simulation of excited states with small populations. The capability of modeling internal energy distributions with little stochastic noise as a function of particle velocity is an important feature of our discrete velocity method.

In the present model, the infinite velocity domain is truncated and discretized giving a finite number of fixed velocities. The mass at each velocity is $\varphi_i(\eta_i, x, t)$, and each such quantity changes due to a stochastic collision model and a finite difference convection operator. A brief overview of the stochastic collision model used is presented in Section 2, and a more detailed method description can be found in either Morris et al. [3] or Clarke's dissertation [4].

Discrete velocity models have been used to simulate gases with rotational and vibrational nonequilibrium in several different works including Tcheremissine [5] and Josyula et al. [6]. Tcheremissine used the discrete ordinate method described in [7] in conjunction with a quantized vibrational and rotational model. A focus was put on approximating the rotational distribution to decrease memory requirements. Reference [6] showed an application of the Anderson et al. model [8] to a discrete velocity framework. A more extensive look at various other discrete velocity models can be found in the text by Aristov [9].

The model described here is built on previous work as described in Morris et al. [3], Clarke et al. [10,11], and Clarke [4]. The scheme was limited to multiple monatomic species. Important developments implemented in our previous work on discrete velocity models include a post-collision remapping scheme with strict mass, momentum, and energy conservation [12], a variance reduced stochastic calculation of the collision integral [13], and methods for multiple species including trace species and species with large mass ratios [11]. The variance reduction method allows one to calculate the collision integral stochastically with greatly reduced noise and/or computation time by operating on deviations from equilibrium instead of the total distribution function [14]. However, there are some subtleties associated with the implementation of a variance reduced method when including internal energy distributions. Hence, variance reduction is not employed for the results presented in this work, and its implementation for diatomic molecules with internal energy states will be presented in a future publication.

The inelastic collision method used in the following work is based on one of the most common approximations used in DSMC, the Larsen–Borgnakke model [15]. The model was originally applied to continuous rotation and vibration distributions [2], but more recent work by Koura [16], Boyd [17], and Bergemann [18] has shown applications to quantized rotation and vibration.

Our objective in this work is to present a low noise discrete velocity method with quantized internal energy that gives accurate, low-noise solutions, particularly for highly excited rotational and vibrational states that have relatively small populations but which contribute significantly to non-equilibrium dissociation rates. In Section 2 a brief outline of the discrete velocity method will be presented followed by the formulation used for quantized internal energies. Next, the collision method will be discussed including collision pair selection, the handling of discrete internal energies (Section 2.1), the mechanics of elastic and inelastic collision depletions (Section 2.2), the implementation of the Larsen–Borgnakke method for discrete internal energies (Section 2.3), and finally the mechanics of replenishing collisions (Section 2.4). In Section 3 we present the results of several test cases for verification purposes. These test cases include three homogeneous relaxation problems and the simulation of a 1-D Mach 12 shock in N_2. Our conclusions and directions for future work are presented in Section 4.

2. Method

Atoms and molecules have a discrete set of internal energy levels [19]. The internal energy states of atoms are the electronic states, and molecules have discrete vibrational and rotational states in addition. In this paper we restrict our considerations to a pure gas of diatomic molecules, and assume they remain in the electronic ground state so that electronic energy states need not be considered explicitly. The rotational and vibrational energy levels can be described using a rotational quantum number denoted by J, the vibrational quantum number v, and the contributions of the nuclear spin and the degeneracy of the rotational level defined by q. Molecular vibrational levels above the ground ($v = 0$) level only begin to become significantly populated at the characteristic vibrational temperature (typically on the order of 10^3 K), but rotational energy levels are excited at much lower temperatures. In fact, most common gas species have a characteristic rotational temperature on the order of 1–5 K. The levels are so closely spaced that at room temperature and above, the rotational distribution is often approximated as a continuous function. However, in this work, discrete, i.e. fully quantized, distributions of both vibrational and rotational energy will be used regardless of the local temperature.