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A physical-based gas–surface interaction model for rarefied gas flow simulation

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ABSTRACT

Empirical gas–surface interaction models, such as the Maxwell model and the Cercignani–Lampis model, are widely used as the boundary condition in rarefied gas flow simulations. The accuracy of these models in the prediction of macroscopic behavior of rarefied gas flows is less satisfactory in some cases especially the highly non-equilibrium ones. Molecular dynamics simulation can accurately resolve the gas–surface interaction process at atomic scale, and hence can predict accurate macroscopic behavior. They are however too computationally expensive to be applied in real problems. In this work, a statistical physical-based gas–surface interaction model, which complies with the basic relations of boundary condition, is developed based on the framework of the washboard model. In virtue of its physical basis, this new model is capable of capturing some important relations/trends for which the classic empirical models fail to model correctly. As such, the new model is much more accurate than the classic models, and in the meantime is more efficient than MD simulations. Therefore, it can serve as a more accurate and efficient boundary condition for rarefied gas flow simulations.

1. Introduction

Rarefied gas flows are widely encountered in modern applications, for example those involving high altitude, low pressure, and micro/nano systems [1]. Driven by the fast development of astronautics, vacuum technology and microelectromechanical systems industry, simulation methods for rarefied gas, such as the direct simulation Monte Carlo method [2], information preservation method [3,4], discrete velocity method and unified gas kinetic scheme [5], have been developed rapidly in the past thirty years. In all these approaches, an indispensable element is the boundary model. Accurate prescription of boundary conditions is the key to ensure the reliability of the simulation results.

Due to the complexity of the microscopic interaction between gas molecules and boundary surface, phenomenological gas–surface interaction models, which are built upon statistically averaged molecular flux distribution, are commonly employed as the boundary conditions in rarefied gas simulations. Currently, the most popular ones are the Maxwell model [6] and Cercignani–Lampis model [7,8]. These models can be generally expressed by scattering kernels which formulate the relation between the velocity distributions of the incident and reflected gas molecule flux at the boundary, and one or two accommodation coefficients are invoked to quantify the momentum or energy exchange between gas and boundary sur-

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face. Several studies [9–14] have tested the performance of these empirical gas–surface interaction models, which revealed several intrinsic limits:

i) Due to the constant accommodation coefficients used for all the incident gas molecules, these empirical models cannot account for the dependence of momentum and energy exchange between gas and boundary surface on the incident conditions such as the energy and the direction of incidence [11,13];

ii) The momentum and energy accommodation coefficients have a fixed functional relation in these empirical models [9,14];

iii) The interplay between gas molecular velocity components is ignored [9,14,15];

iv) They fail to produce the intricate pattern of scattering velocity distribution observed in experiments and molecular dynamics (MD) simulations [11,13].

These limits of the classic empirical gas–surface interaction models greatly impair the accuracy of the rarefied gas flow simulations [14].

To develop better gas–surface interaction models, some researchers resorted to mathematical modeling. According to the basic relations of boundary conditions, which include the non-negativity, normalization and reciprocity relations, mathematical models with more sophisticated scattering kernels, such as combination of classic empirical models [11,13,15] and employing velocity dependent accommodation coefficients [16], have been developed. However, this approach inevitably introduces more adjustable parameters, which are difficult to be obtained in practice. Consequently, these new mathematical models are difficult to be applied in rarefied gas flow simulations, though they were suggested to possess higher accuracy.

Physical modeling is an alternative approach to develop better gas–surface interaction models. Since 1960, a serial of physical models, including the hard cube model, soft cube model and washboard model, have been developed to qualitatively capture the scattering phenomena observed in molecular beam experiments [17–22]. The basic idea of these physical models is to simplify the complex gas–surface interaction as elastic binary collisions between gas molecules and effective surface cubes. Among these models, the washboard model [20–22] is the most sophisticated one that incorporates attractive potential well, anisotropic response of the surface and three dimensional surface roughness. Using only three effective physical parameters, which are the surface roughness A, the attractive potential well depth W and surface cube mass M, the washboard model is able to capture complex microscopic interaction phenomena, such as the interplay between gas molecular velocity components, trapping and desorption. It has been demonstrated that the washboard model can reproduce the angular and energy distributions of reflected gas molecule flux obtained in MD simulations as well as the reduced force coefficients measured in experiments [20–22]. However, most physical models do not satisfy the basic relations of boundary condition, especially the reciprocity relation [23,24]. As a result, these physical models violate the H-theorem.

An accurate physical approach to model gas–surface interaction is MD simulation. MD simulation resolves the microscopic dynamics of gas–surface interaction accurately, and has been successfully employed as the boundary condition in hybrid simulation scheme for rarefied gas flow [25–27]. However, it is well known that the computational cost of MD simulation is extremely high, which prohibits its practical use. A new physical-based gas–surface interaction model, which is more efficient than MD simulation, has been developed and is presented. This model complies with the basic relations of boundary condition, overcomes some intrinsic limits of the classic empirical gas–surface interaction models, and hence is more accurate.

The organization of the paper is as follows. Section 2 reviews the basic relations of boundary condition and two classic empirical gas–surface interaction models. Section 3 introduces the washboard model and points out its deficiency. The new physical-based gas–surface interaction model is presented next. Section 5 demonstrates the advantages of the new model with respect to the limits of the classic empirical gas–surface interaction models. Summary of the work is given in the last section.

2. Basic relations of the boundary conditions and the classic empirical gas–surface interaction models

In rarefied gas flow simulation, the boundary condition prescribes the relation between the incident and reflected gas molecular velocity distributions, f_{in} and f_{re}, at the boundary surface. It can be expressed generally via the scattering kernel $\mathcal{R}(\mathbf{v}' \to \mathbf{v})$ as,

$$v_n f_{\text{re}}(\mathbf{v}) = \int_{v_n'<0} |v_n'| f_{\text{in}}(\mathbf{v}') \mathcal{R}(\mathbf{v}' \to \mathbf{v}) d\mathbf{v}' \tag{1}$$

where $\mathbf{v}'$ and $\mathbf{v}$ are the velocities of the incident and reflected gas molecules, respectively. $v_n' = \mathbf{v}' \cdot \mathbf{N} < 0$ and $v_n = \mathbf{v} \cdot \mathbf{N} > 0$ are their velocity components normal to the boundary surface with the global surface normal $\mathbf{N}$ pointing into the gas. The scattering kernel $\mathcal{R}(\mathbf{v}' \to \mathbf{v})$ denotes the probability density of a molecule impinging on the surface with a velocity of $\mathbf{v}'$ and being reflected with a new velocity in the interval of $\{\mathbf{v}, \mathbf{v} + d\mathbf{v}\}$. The scattering kernel must obey the non-negativity, normalization and reciprocity relations as,

$$\mathcal{R}(\mathbf{v}' \to \mathbf{v}) \geq 0 \tag{2}$$

$$\int_{v_n>0} \mathcal{R}(\mathbf{v}' \to \mathbf{v}) d\mathbf{v} = 1 \tag{3}$$