Langmuir–Maxwell and Langmuir–Smoluchowski boundary conditions for thermal gas flow simulations in hypersonic aerodynamics

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ABSTRACT

The simulation of nonequilibrium thermal gas flow is important for the aerothermodynamic design of re-entry and other high-altitude vehicles. In computational fluid dynamics, the accuracy of the solution to the Navier–Stokes–Fourier (N–S–F) equations depends on the accuracy of the surface boundary conditions. We propose new boundary conditions (called the Langmuir–Maxwell and the Langmuir–Smoluchowski conditions), for use with the N–S–F equations, which combine the Langmuir surface adsorption isotherm with the Maxwell/Smoluchowski slip/jump conditions in order to capture some of the physical processes involved in gas flow over a surface. These new conditions are validated for flat plate flow, circular cylinder in cross-flow, and the flow over a sharp wedge for Mach numbers ranging from 6 to 24, and for argon and nitrogen as the working gases. Our simulation results show that the new boundary conditions give better predictions for the surface pressures, compared with published experimental and DSMC data.

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1. Introduction

Translational nonequilibrium of a rarefied gas flow can be characterized by the Knudsen number, Kn, which is the ratio of the gas molecular mean free path λ (i.e. the average distance a molecule travels between successive intermolecular collisions) to a characteristic length of an aerodynamic vehicle body, l. In order for the Navier–Stokes–Fourier (N–S–F) equations, as generally used in Computational Fluid Dynamics (CFD) to produce reasonable results in the Kn range up to 0.1, velocity slip and temperature jump boundary conditions should be applied at the surface.

The first-order conventional slip condition was developed by Maxwell for a flat plate [1]. It remains the simplest and most useful description of the slip condition, and depends on the normal gradient of velocity at the surface and a thermal creep term. The first-order slip condition described by Shen et al. [2] was derived using the Chapman–Enskog solution of the Boltzmann equation under the relaxation time approximation. In this condition, the slip velocity depends not only on the velocity gradient in the surface-normal direction but also on the pressure gradient in the flow direction. A general slip condition for a solid surface in rarefied multi-compo-

nent gas flows has been reported by Zade et al. [3]. The slip condition developed by Gökçen and MacCormack [4] aims to reduce to the classical Maxwell slip condition in the continuum limit, and yield the correct shear stress in free molecular flow in the limiting case of very large Knudsen numbers. All these first-order slip conditions make use of a free parameter in the slip equation, namely the tangential momentum accommodation coefficient σ_u. This varies between 0 and 1, and determines the proportion of molecules reflected from the surface specularly $(1 - \sigma_u)$ or diffusely σ_u.

Second-order slip boundary conditions have also been developed [5–8]. These include an additional second-order term in the normal gradient of velocity. Our simulation results in [9] showed that using the second-order slip condition is not much better than using the conventional Maxwell slip condition, when simulating thermal gas flows in hypersonic aerodynamics.

The temperature jump condition developed by Smoluchowski [10] is driven by the heat flux to the surface in the normal direction. A general temperature jump condition for rarefied multi-component gas flows is also described by Zade et al. [3]. Gökçen and MacCormack [4] proposed a temperature jump condition both to simplify the Smoluchowski jump condition, and to yield the correct heat transfer in free molecular flow in the limiting case of very large Knudsen numbers. These temperature jump conditions also depend on a free parameter, namely the thermal accommodation coefficient σ_T, which varies between 0 and 1, with 1 for a perfect energy exchange between gas molecules and solid surfaces, and 0 corresponding to no energy exchange.

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