DSMC-Based Shear-Stress/Velocity-Slip Boundary Condition for Navier-Stokes Couette-Flow Simulations

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Abstract. Direct Simulation Monte Carlo (DSMC) simulations are used to develop a shear-stress/velocity-slip boundary condition for Navier-Stokes (NS) simulations of low-speed isothermal Couette flow. In this boundary condition, the wall shear stress equals the product of the difference between the gas and wall velocities and a momentum transfer coefficient. This momentum transfer coefficient depends on two dimensionless parameters that determine its behavior in the near-continuum and transitional regimes, respectively. For a given gas, these parameters are determined by comparing the NS Couette-flow shear-stress expression to DSMC shear-stress values for free-molecular to near-continuum pressures with three values of the accommodation coefficient. The parameter values for argon, helium, nitrogen, air, and inverse-power-law (IPL) interactions from hard-sphere to Maxwell lie within narrow ranges. For the hard-sphere interaction, the DSMC-based results are in excellent agreement with previously published analytical approximations.

Keywords: Direct Simulation Monte Carlo, Couette flow, shear stress, velocity slip, Navier-Stokes equations
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INTRODUCTION

Microelectromechanical systems (MEMS) often employ gears to transmit mechanical action (Figure 1, left [1]). Such gears can be 100-1000 μm in diameter and are separated from the adjacent motionless parallel substrate by a narrow gap 1-10 μm in height. When the gear rotates steadily, the gas within the gap away from the edges can be described approximately as locally being in Couette flow (Figure 1, right, offset so as to have zero average velocity). The different tangential velocities of the gear and the substrate produce a shear stress within the gas that produces a resistive torque on the gear. In ambient air, the molecular mean free path is about 0.06 μm, which is not negligible compared to the gap height, and at reduced pressures sometimes encountered in packaging, the mean free path is proportionally larger. Therefore, noncontinuum effects must be considered when computing the gas shear stress.

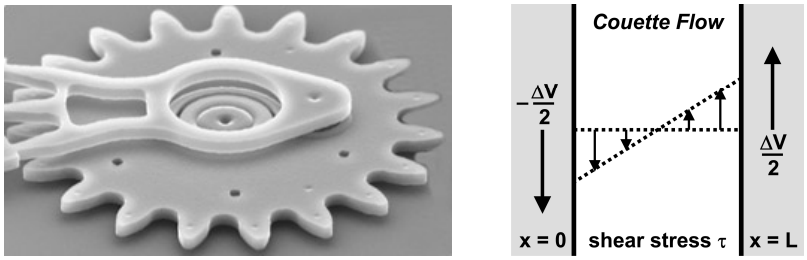

FIGURE 1. Left: MEMS gear adjacent to substrate [1]. Right: Schematic diagram of Couette flow.

Simple expressions for the shear stress encountered in noncontinuum Couette flow that interpolate between the free-molecular and continuum limits have been known for decades [2]. However, these expressions are less accurate in the transitional and near-continuum regimes and in particular do not account accurately for the noncontinuum effects in these regimes. In the following sections, Direct Simulation Monte Carlo (DSMC) [3] simulations are used to develop a boundary condition for Navier-Stokes (NS) simulations of Couette flow that produces accurate values of the shear stress in all flow regimes: continuum, near-continuum, transitional, and free-molecular.

NS BOUNDARY CONDITION FOR COUETTE FLOW

Most attempts to develop more accurate boundary conditions for NS simulations of Couette flow have involved including higher-order spatial derivatives of the gas velocity in the expression for the slip velocity, which is the difference between the wall and gas velocities [4,5], with the goal of producing accurate velocity profiles and shear stresses. This approach is not followed here. Instead, an approach like that of Gallis et al. [6] for heat transfer is followed. The basis of their approach is that, from an engineering point of view in MEMS design, it is of primary importance to accurately predict the gas-phase transfer of energy and momentum between the solid objects and only of secondary importance to accurately predict temperature and velocity profiles within the gas itself. Thus, they equate the conduction heat flux in the gas adjacent to a solid object (a "wall") to the product of the difference between the solid and gas temperatures and a heat transfer coefficient prescribed to produce the correct behavior in all limiting regimes. They show that this approach produces accurate heat fluxes but only approximate temperature profiles in the gas. The same type of approach is followed here for gas-phase momentum transfer in Couette flow. Thus, the wall shear stress τ_{wall} is taken to be equal to the product of the difference between the gas and wall tangential velocities, v and V_{wall}, respectively, and a momentum transfer coefficient k, which is defined to depend on the tangential momentum accommodation coefficient σ, the system Knudsen number Kn, and two positive order-unity dimensionless parameters d_1 and d_2:

$$\tau_{\text{wall}} = \mu\frac{\partial v}{\partial n} = k\left(v - V_{\text{wall}}\right),\ k = \frac{\sigma\rho c_0}{S_1 S_2},\ S_1 = 2-\sigma,\ S_2 = 1+\frac{d_1\sigma}{1+d_2\text{Kn}},\ \text{Kn} = \frac{\lambda}{L};$$
$$\lambda = \frac{\mu}{\rho c_0},\ c_0 = \frac{\bar{c}}{2} = \sqrt{\frac{2k_B T}{\pi m}},\ \rho = mn = \frac{mp}{k_B T}. \tag{1}$$

Here, L is the wall separation (Figure 1), λ is the mean free path (as defined here), μ is the viscosity, c_0 is half the mean molecular speed $\bar{c}$, ρ is the mass density, p is the pressure, T is the temperature, m is the molecular mass, and k_B is the Boltzmann constant. This boundary condition has the following limits in the indicated regimes:

$$\text{Kn} >> 1,\ 0 \le \sigma \le 1,\ S_1 = 2-\sigma,\ S_2 = 1,\ \tau_{\text{wall}} = \left(\frac{\sigma}{2-\sigma}\right)\left(\frac{mn\bar{c}}{4}\right)\Delta V;$$
$$\text{Kn} << 1,\ \sigma << 1,\ S_1 = 2,\ S_2 = 1,\ \tau_{\text{wall}} = \sigma\left(\frac{mn\bar{c}}{4}\right)\left(v - V_{\text{wall}}\right);$$
$$\text{Kn} << 1,\ \sigma = 1,\ S_1 = 1,\ S_2 = 1+d_1,\ \left(1+d_1\right)\lambda\frac{\partial v}{\partial n} = v - V_{\text{wall}};$$
$$\text{Kn} \to 0,\ \sigma = 0,\ \tau_{\text{wall}} = \mu\frac{\partial v}{\partial n} = 0;\ \text{Kn} \to 0,\ 0 < \sigma \le 1,\ v = V_{\text{wall}}. \tag{2}$$

For free-molecular flow with arbitrary accommodation ($\text{Kn} >> 1,\ 0 \le \sigma \le 1$), the wall shear stress corresponds to the value found by matching two rightward and two leftward half-range Maxwellians with velocities $\pm\Delta V/2$ (Figure 1). For near-continuum flow with small accommodation ($\text{Kn} << 1,\ \sigma << 1$), the wall shear stress corresponds to the value from reflecting a small fraction σ of a half-range Maxwellian with velocity v into a half-range Maxwellian traveling oppositely with velocity V_{wall}. For near-continuum flow with unity accommodation ($\text{Kn} << 1,\ \sigma = 1$), the common form of the slip boundary condition is obtained [4,5], suggesting that $d_1 \approx 0.1\text{-}0.2$ represents the Knudsen layer, depending on the details of the molecular interaction. For continuum flow with zero accommodation ($\text{Kn} \to 0,\ \sigma = 0$), the zero-shear-stress or symmetry boundary condition is obtained. For continuum flow with nonzero accommodation ($\text{Kn} \to 0,\ 0 < \sigma \le 1$), the no-slip boundary condition is obtained. The NS equations and boundary condition have a closed-form expression for the Couette-flow wall shear stress, in which d_1 affects the near-continuum regime ($\text{Kn} << 1$) and d_2 affects the transitional regime ($\text{Kn} \approx 1$):

$$\frac{\tau_{\text{wall}}}{\tau_{\text{cont}}} = \frac{1}{1+\left(2S_1 S_2 \text{Kn}/\sigma\right)},\ \tau_{\text{cont}} = \frac{\mu\Delta V}{L},\ S_1 = 2-\sigma,\ S_2 = 1+\frac{d_1\sigma}{1+d_2\text{Kn}},\ \text{Kn} = \frac{\lambda}{L}. \tag{3}$$

DSMC SIMULATIONS OF NONCONTINUUM COUETTE FLOW

DSMC simulations are performed for the Couette-flow geometry shown in Figure 1 with physical and numerical parameters shown in Table 1. The Variable Soft Sphere (VSS) model is used to represent molecular collisions [3], where the reference diameter d_{ref} depends on ω and α, the viscosity ratio μ_∞/μ_1 [7], and reference quantities:

$$d_{\text{ref}} = \left(\frac{5(\alpha+1)(\alpha+2)(mk_B T_{\text{ref}}/\pi)^{1/2}}{4\alpha(5-2\omega)(7-2\omega)\mu_{\text{ref}}(\mu_1/\mu_\infty)} \right)^{1/2} . \tag{4}$$

In all cases, the wall separation is 1 mm, the wall velocities are ±10 m/s, the accommodation coefficient is one of 1.00, 0.50, or 0.25, and the pressure is one of 13 values distributed approximately logarithmically between 10^{-1} Pa and 10^{3} Pa. Thus, the gas velocities are extremely small compared to the mean molecular speed, so viscous heating is very small, and the flows are nearly isothermal. In all simulations, the cell size is smaller than the mean free path, the time step is smaller than the collision time, the average move is smaller than the cell size, and the time at which steady-state averaging is begun is much larger than the ballistic time and the maximum diffusion time. Two sets of simulations are performed. In the first, argon, helium, nitrogen, and air with properties from Bird [3] are examined. In the second, a gas with the mass and reference viscosity of argon but with different values of the VSS parameters ω and α is examined, where ω is varied from 0.5 (the hard-sphere interaction) to 1.0 (the Maxwell interaction) in increments of 0.1 and α is assigned either the Variable Hard Sphere (VHS) value of 1.0 or the Inverse-Power-Law (IPL) value [7], which varies from 1.0 to 2.13986 over the above range for ω.

TABLE 1. Physical and numerical parameters used in analysis and simulations, many of which are from Bird [3].

Property	Symbol	Argon	Helium	Nitrogen	Air
Boltzmann constant	k_B	1.380658×10^{-23} J/K	1.380658×10^{-23} J/K	1.380658×10^{-23} J/K	1.380658×10^{-23} J/K
Molecular mass	m	66.3×10^{-27} kg	6.65×10^{-27} kg	46.5×10^{-27} kg	48.1×10^{-27} kg
Temperature, reference	T_{ref}	273.15 K	273.15 K	273.15 K	273.15 K
Viscosity, reference	μ_{ref}	2.117×10^{-5} Pa·s	1.865×10^{-5} Pa·s	1.656×10^{-5} Pa·s	1.719×10^{-5} Pa·s
Viscosity temperature expon.	ω	0.81	0.66	0.74	0.77
Angular scattering exponent	α	1.40	1.26	1.36	1.37
Infinite-first viscosity ratio	μ_∞/μ_1	1.002277	1.007339	1.004275	1.003342
Number of rotational modes	ζ_{rot}	0	0	2	2
Rotational collision number	Z_{rot}	-	-	5	5
Temperature	T	273.15 K	273.15 K	273.15 K	273.15 K
Pressure	p	10^{-1}-10^{3} Pa	10^{-1}-10^{3} Pa	10^{-1}-10^{3} Pa	10^{-1}-10^{3} Pa
Mass density at $p=10^2$ Pa	ρ	1.758×10^{-3} kg/m^3	1.763×10^{-4} kg/m^3	1.233×10^{-3} kg/m^3	1.275×10^{-3} kg/m^3
Mean molecular speed	$\bar{c}$	380 m/s	1200 m/s	454 m/s	446 m/s
Mean free path at $p=10^2$ Pa	λ	63.3 μm	176 μm	59.2 μm	60.5 μm
Collision time at $p=10^2$ Pa	t_0	167 ns	147 ns	130 ns	136 ns
Accommodation coefficient	σ	1.00, 0.50, 0.25	1.00, 0.50, 0.25	1.00, 0.50, 0.25	1.00, 0.50, 0.25
Velocity difference	ΔV	20 m/s	20 m/s	20 m/s	20 m/s
Wall separation	L	1 mm	1 mm	1 mm	1 mm
Cell size at $p\le10^2$ Pa	Δx	10 μm	10 μm	10 μm	10 μm
at 10^2 Pa < $p\le10^3$ Pa		2.5 μm	2.5 μm	2.5 μm	2.5 μm
Time step at $p\le10^2$ Pa	Δt	7 ns	7 ns	7 ns	7 ns
at 10^2 Pa < $p\le10^3$ Pa		3.5 ns	1.75 ns	3.5 ns	3.5 ns
Average move at $p\le10^2$ Pa	$\bar{c}\Delta t$	2.7 μm	8.4 μm	3.2 μm	3.1 μm
at 10^2 Pa < $p\le10^3$ Pa		1.3 μm	2.1 μm	1.6 μm	1.6 μm
Number of simulators per cell	N_s	30	30	30	30
Ballistic time	$L/\bar{c}$	0.0026 ms	0.0008 ms	0.0022 ms	0.0022 ms
Diffusion time at $p=10^3$ Pa	$\rho L^2/\mu$	0.83 ms	0.09 ms	0.74 ms	0.74 ms
Steady-state initiation time	t_s	7 ms	7 ms	7 ms	7 ms

Figure 2 (left) shows velocity fields from the first set of DSMC simulations for argon with unity accommodation and properties from Table 1. At the highest pressure, the velocity profile is linear with small discontinuities at the walls, as expected for near-continuum flow, whereas, at the lowest pressure, the velocity profile is nearly zero, as expected for free-molecular flow. Figure 2 (right) shows the corresponding NS velocity profiles based on Equation (3) for parameter values of $d_1 = 0.164$ and $d_2 = 0.568$, which are determined in the following manner.

Figure 3 (upper left, circles) shows the shear-stress values corresponding to the DSMC argon velocity profiles with unity accommodation (shown in Figure 2) and with non-unity accommodation (not shown in Figure 2, but qualitatively similar). Additionally, Figure 3 (upper left, curves) shows the argon shear-stress values from the NS expression, Equation (3), for which the parameters d_1 and d_2 have been adjusted so that the logarithms of the NS values achieve the best match to the logarithms of the DSMC values in the least-squares sense. The parameter values thus determined for argon, $d_1 = 0.164$ and $d_2 = 0.568$, are shown in the lower-right corner of the shear-stress plot. From Figures 2 and 3, the shear-stress values are seen to be more accurately represented than the velocity profiles.

Figure 3 also shows the results from this procedure for the other three gases considered: helium (upper right), nitrogen (lower left), and air (lower right). The parameters for all four gases lie within narrow ranges that are similar to the uncertainties estimated from the fits, $\Delta d_1 = 0.02$ and $\Delta d_2 = 0.06$. Additionally, their values are very close to the values of the analogous parameters in the heat transfer coefficient of Gallis et al. [6].

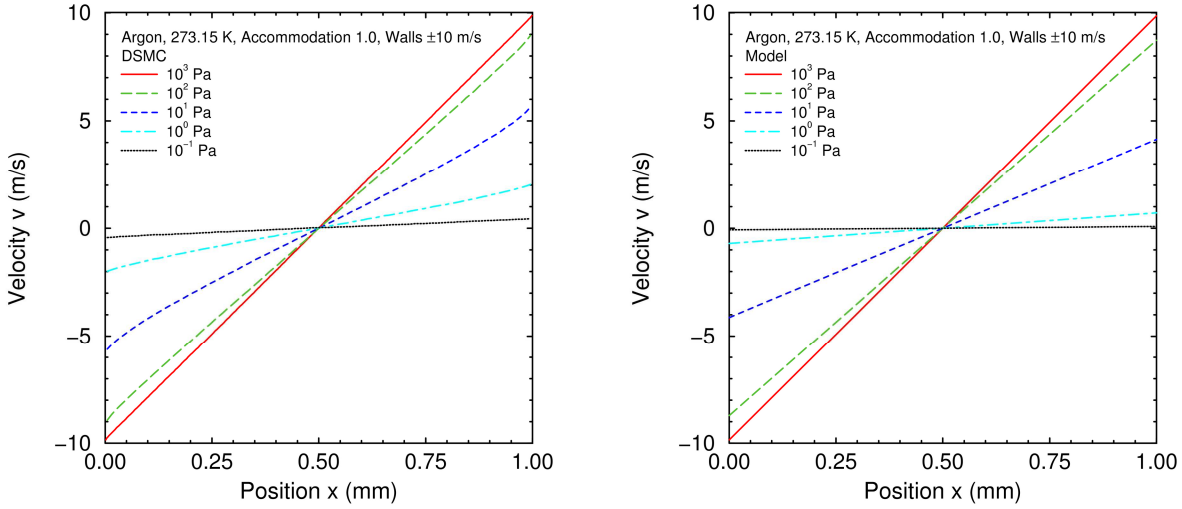

FIGURE 2. Couette-flow velocity profiles at different pressures. Left: DSMC simulations. Right: NS expression.

Given the narrow ranges of values for the parameters d_1 and d_2, a second set of DSMC simulations is performed to quantify the dependence of these parameters on the VSS parameters ω and α. Figure 4 (left) shows the values of α vs. ω for common gases from Bird [3] and the corresponding VHS and IPL values [7], which are seen to bound the values for common gases. Therefore, this second set of simulations uses the argon properties of Table 1 except that ω is varied from 0.5 to 1.0 and α is assigned to either the VHS value or the IPL value. Figure 4 (right) shows the boundary-condition parameters from both sets of DSMC simulations, where the error bars indicate the uncertainties discussed above. The parameters d_1 and d_2 depend weakly on the VSS parameters ω and α, exhibiting very slight increasing trends with ω that lie almost within the error bars. In fact, the values in this figure can be represented by the expressions $d_1 = 0.15 \pm 0.02$ and $d_2 = 0.59 \pm 0.07$, despite the fact that nitrogen and air both have two fully excited rotational energy modes (see Table 1). The helium d_2 value is slightly higher than most of the other d_2 values, but the difference is similar to the uncertainty.

Figure 5 plots the nondimensional momentum transfer coefficient $k/\rho c_0$ vs. the accommodation coefficient for hard-sphere molecules as determined from the DSMC-based expression and from six analytical approximations of Siewert and Sharipov [8]. By construction, both approaches have $k/\rho c_0 \to \sigma/2$ as $\sigma \to 0$, so the good agreement in this regime is expected. As $\sigma \to 1$, the DSMC-based expression has $k/\rho c_0 \to 1/(1+d_1)$, so the good agreement in this regime indicates that the DSMC value of d_1 for hard-sphere molecules is accurate. Additionally, the uncertainty in the DSMC value of $\Delta d_1 = 0.02$ would produce a variation in the DSMC values comparable to the variation observed between the six approximations presented in Siewert and Sharipov [8].

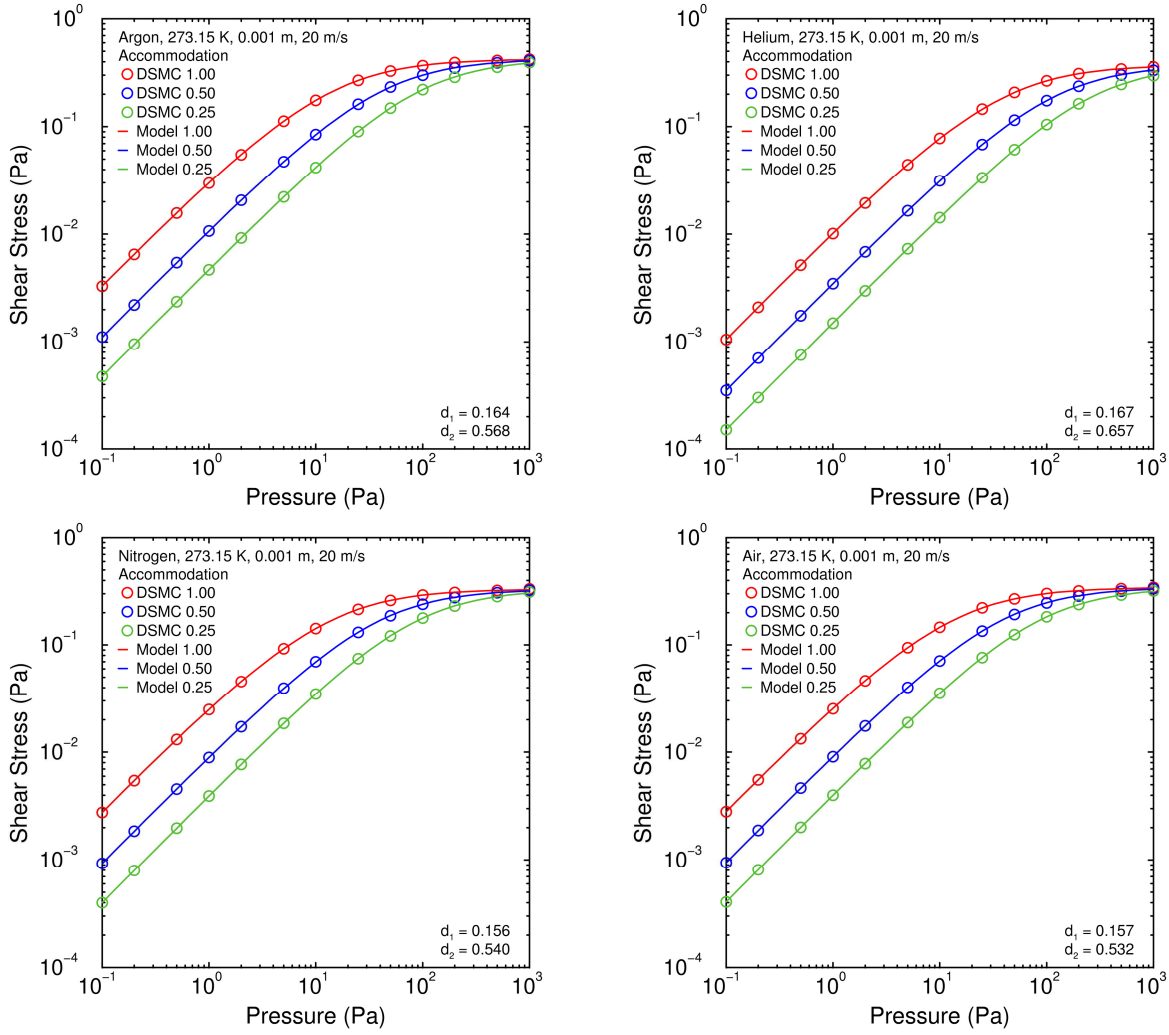

FIGURE 3. Comparison of DSMC and NS shear-stress values for argon, helium, nitrogen, and air.

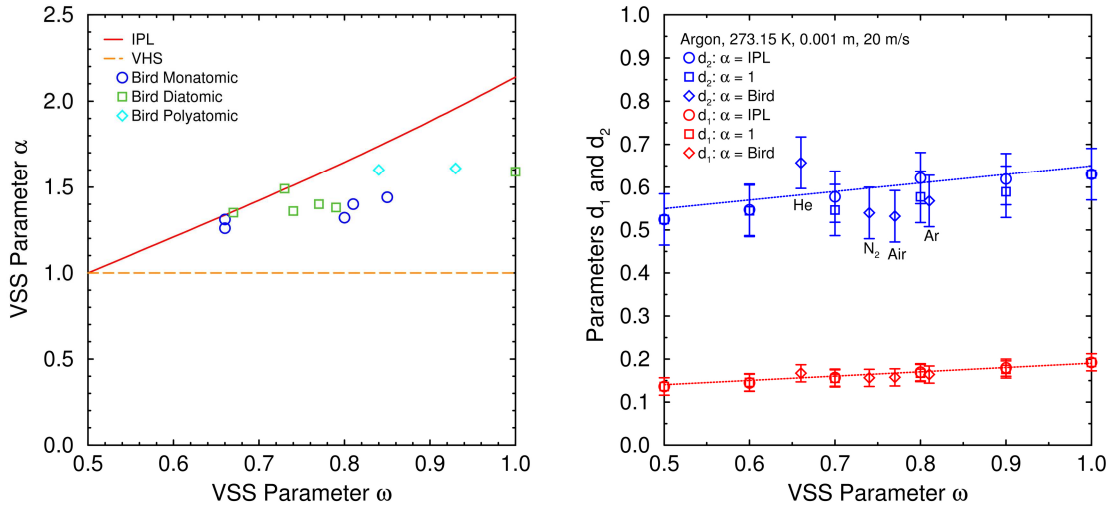

FIGURE 4. Left: VSS parameters for common gases [3,7]. Right: Parameters for various values of VSS parameters.

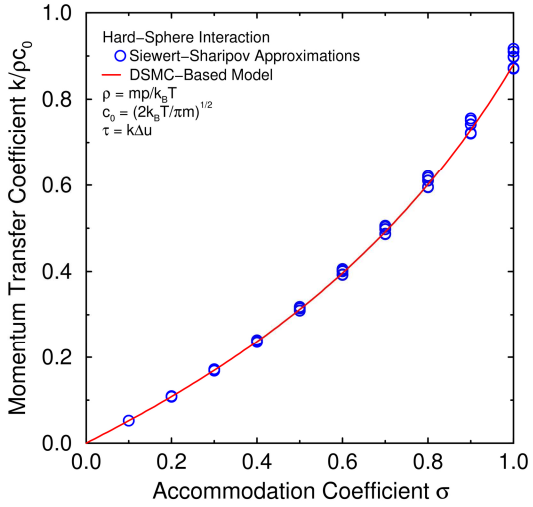

FIGURE 5. DSMC and approximate values [8] for the momentum transfer coefficient of a hard-sphere gas.

CONCLUSIONS

The Direct Simulation Monte Carlo (DSMC) method is used to simulate isothermal low-speed steady Couette flow from almost free-molecular to near-continuum conditions for several values of the accommodation coefficient. Navier-Stokes (NS) shear-stress values based on a shear-stress/velocity slip boundary condition are compared to the corresponding DSMC values to determine the best-fit values for the two dimensionless parameters in this boundary condition. For argon, helium, nitrogen, air, and all VHS and IPL gases represented by the VSS interaction, the values of these parameters lie within narrow ranges comparable to the uncertainties in their values. The value of one of these parameters is in good agreement with values obtained from analytical approximations for the hard-sphere interaction. The resulting boundary condition is suitable for NS simulations of Couette flows in MEMS geometries, and the corresponding closed-form expression for the wall shear stress is suitable for estimating the gas-phase torque on rotating MEMS gears or the gas-phase force on sliding parallel MEMS parts.

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