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## Anomalous flow profile due to the curvature effect on slip length

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Einzel, Panzer, and Liu [Phys. Rev. Lett. **64**, 2269 (1990)] suggest that the slip boundary condition for a fluid moving near a wall is modified by the radius of curvature of the surface. Using particle simulations of a microscopic flow between concentric cylinders we qualitatively confirm their prediction and point out that the effect is seen in a limiting case derived by Maxwell [Nature (London) **16**, 244 (1877)].  
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In conventional hydrodynamics, one assumes the no-slip boundary condition for a fluid moving past a solid wall, that is, the velocity of the fluid at the surface is assumed to equal the wall's velocity. As was originally pointed out by Maxwell [1,2], this boundary condition is not accurate at microscopic scales since gradients normal to the surface cause particles approaching the wall to have a different velocity distribution from those leaving the wall. For a fluid moving past a stationary wall, this "slip" phenomenon is expressed by the boundary condition,  $v_{\parallel} = \zeta \hat{\mathbf{n}} \cdot \nabla v_{\parallel}$ , where  $v_{\parallel}$  is the component of fluid velocity parallel to the surface,  $\hat{\mathbf{n}}$  is a unit vector normal to the surface, and  $\zeta$  is the slip length. The velocity profile extrapolates to zero at a distance  $\zeta$  inside the wall. For a dilute gas moving over a plane, the slip length is [3],  $\zeta_0 = a(2 - \alpha/\alpha)\lambda$ , where  $\lambda$  is the mean free path and  $a \approx 1.15$ . The accommodation coefficient  $\alpha$  is the fraction of molecules whose velocity is thermalized at the surface and  $(1 - \alpha)$  is the fraction that scatters elastically. In a planar channel (flow between parallel planes), the slip length at one wall is affected by the presence of the other wall when the width of the channel is less than about  $10\lambda$  [4,5].

Einzel, Panzer, and Liu (EPL) [6,7] have suggested a more general form for the slip length,  $\zeta = (1/\zeta_0 - 1/\rho)^{-1}$ , where  $\rho$  is the radius of curvature of the surface ( $\rho > 0$  for a concave surface). As an example, EPL predict the angular speed for a fluid between concentric cylinders (radii  $R_1$  and  $R_2$ ,  $R_1 < R_2$ ) to be

$$v_{\theta} = \frac{\omega}{A - B} \left( Ar - \frac{1}{r} \right), \quad (1)$$

where

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$$A = \frac{1}{R_2^2} \left( 1 - 2 \frac{\zeta_0}{R_2} \right); \quad B = \frac{1}{R_1^2} \left( 1 + 2 \frac{\zeta_0}{R_1} \right), \quad (2)$$

and  $\omega$  is angular frequency of the inner cylinder; the outer cylinder is stationary. When  $\zeta_0$  is large, EPL point out that the velocity field extrapolates to zero in the fluid and not, as usual, behind the outer wall [7].

We performed simulations of a hard sphere dilute gas between concentric cylinders in order to test these predictions. Because of its computational efficiency, the direct simulation Monte Carlo (DSMC) method was employed [8,9]. As in molecular dynamics (MD), the DSMC algorithm evolves the positions and velocities of the gas particles. Unlike MD, the individual collision trajectories are not calculated, instead collisions are stochastically selected and evaluated using the rates and probabilities given by kinetic theory. Previous studies have demonstrated DSMC to be in excellent agreement with laboratory experiments [10] and MD simulations [11], including predictions of slip in planar geometries [5].

A number of DSMC simulations were performed, but here we present only the results from various runs for a system of 51 200 hard sphere particles between concentric cylinders with  $R_1 = 3\lambda$ ,  $R_2 = 5\lambda$ ,  $\lambda = 6.25 \times 10^{-8}$  m,  $\omega = 5.17 \times 10^8$  rad/s. The simulations modeled argon at STP conditions; the variation in density and temperature across the system was less than 1% and 3%, respectively. The sound speed is 322 m/s and in all cases the flow is subsonic.

The DSMC simulation results for the angular speed, shown in Figs. 1 and 2, are in qualitative agreement with Eq. (1). As predicted by EPL, when the accommodation is low, the velocity profile reverses slope so that the gas moves fastest near the stationary outer wall. Quantitative agreement was not expected since the separation between the cylinder walls is only two mean free paths. We find quantitative agreement when the system size is increased but then the curvature effect is less dramatic and the reversal of the  $v_{\theta}$  profile cannot be obtained.

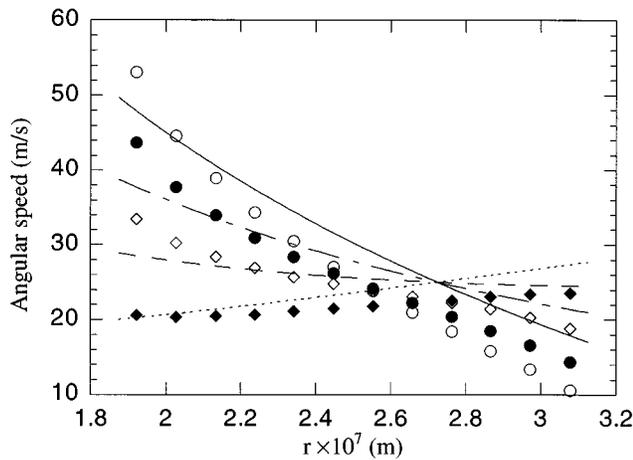


FIG. 1. Angular speed of the gas vs radial distance; points are from the DSMC simulation, lines are the EPL prediction, Eq. (1). Surface accommodation is  $\alpha = 1.0$  (open circles; solid line);  $0.7$  (filled circles; dashed-dotted line);  $0.4$  (open diamonds; dashed line);  $0.1$  (filled diamonds; dotted line).

Finally, for the case where  $\alpha \rightarrow 0$  (total specular reflection at the walls) Maxwell [12] predicted that the gas should rotate as a solid body ( $v_\theta \propto r$ ) at constant temperature and his prediction is confirmed by the simulations (see Fig. 2).

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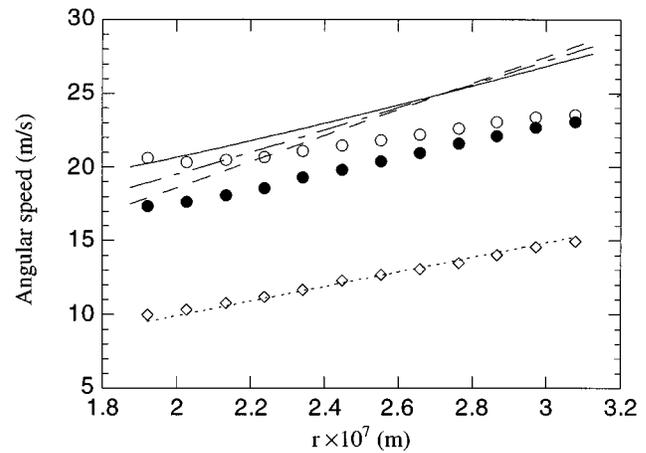


FIG. 2. Angular speed of the gas vs radial distance; points are from the DSMC simulation, upper three lines are the EPL prediction, Eq. (1). Surface accommodation is  $\alpha = 0.1$  (open circles; solid line);  $0.05$  (filled circles; dashed-dotted line);  $0.01$  (open diamonds; dashed line). Dotted line is the velocity profile for solid body rotation (as fit to the data for  $\alpha = 0.01$ ).

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