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# A Kinetic Model for Gas-Surface Interaction

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## ABSTRACT

Fluid-wall interaction plays an important role in determining the properties of micro/nanoflows[1]. In regions where the fluid is in contact with a solid boundary, temperature jumps and velocity slip produce deviations from the ordinary hydrodynamic behaviour of the fluid[2]. When dealing with dilute gases[2], the characteristic space and time scales are much larger than molecular sizes and molecular interaction times, respectively. Hence, gas-wall interaction modeling can be based on the assumption that the solid boundary is a smooth, structureless and impenetrable surface whose action on the gas distribution function can be described by a scattering kernel. The determination of the kernel structure from first principles would require solving the complex dynamics of a fluid molecule in interaction with wall molecules, therefore the scattering kernel expressions are more often based on phenomenological models[2]. The need to give physically sound bases to gas-surface interaction model and to relate model parameters to the basic physical properties of molecular interaction has triggered a number of studies in which molecular dynamics (MD) techniques have been used to investigate atomic or molecular scattering from solids[3-5]. However, the coupling of MD to Monte Carlo simulations of dilute gases is computationally expensive. The aim of the present work is to formulate and validate a kinetic model of a monatomic fluid interacting with a solid wall. It is assumed that interatomic forces can be derived from a potential which results from the superposition of a repulsive hard sphere contribution and a soft tail. The adoption of simplifying assumptions about pair correlations leads to a linear Enskog-Vlasov kinetic equation which can be easily solved by the same Monte Carlo scheme used to calculate the fluid motion, thus avoiding hybrid schemes. It is shown that the model predictions are in good agreement with MD simulations[6]. Moreover, the effects of non-local re-emission on drag coefficients of nano-particles are discussed.

## REFERENCES


[1] G. E. Karniadakis, N. Aluru, A. Beskok: *Microflows and nanoflows : fundamentals and simulation* (Springer, 2005)

[2] C. Cercignani: *The Boltzmann Equation and Its Applications* (Springer, 1988)

[3] M. Cieplak, J. Koplik, J. R. Banavar: *Physical Review Letters* **86** (2001)

[4] K. Yamamoto, H. Takeuchi, T. Hyakutake: *Rarefied Gas Dynamics:* $23^{rd}$ *International Symposium* (AIP, 2003)

[5] K. Yamamoto, H. Takeuchi, T. Hyakutake: *Physics of Fluids* **18** (2006)

[6] A. Frezzotti, L. Gibelli: *JMES* **222** (2008)