Transport Coefficients of a Rarefied Gas in a Hydrophobic Nanopore

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While Knudsen diffusion of rarefied gases in small cylindrical pores, isothermal as well as non-isothermal, is a well-studied phenomenon, we provide an analytical model to assess the effect of a repulsive interaction between the gas particles and the pore walls. Isothermal transport of rarefied gases has seen some recent advances in this direction [1], as well as the non-isothermal case for slip flow [2]. We provide analytical expressions for the thermal conductivity, the gas permeability, and the heat-mass coupling coefficients, as functions of the range and strength of the hydrophobic interaction. The expressions are shown to reduce to those of ordinary Knudsen diffusion as the interaction vanishes, and the correction terms are each given physical interpretations based on their effects on the average gas density profile and on the flight paths of the particles. We show also how these transport coefficients are incorporated into the overall transport coefficients of a composite system of which the cylindrical pore is one of the parts. This is relevant for building analytical models for transport through more complicated porous media.

References

[1] Bhatia el at. Molecular transport in nanopores: a theoretical perspective. Phys. Chem. Chem. Phys., 2011, 13, 15350-15383.

[2] K. Proesmans and D. Frenkel. Comparing theory and simulation for thermo-osmosis. J. Chem. Phys., 151:124109, 2019.