Thermal Transport of Two Layers of Carbon Dioxide in a Carbon Membrane from Non-Equilibrium Molecular Dynamics

Thuat T. Trinh [C, S], Dick Bedeaux and Signe Kjelstrup
Chemistry Dept., Norwegian University of Science and Technology, Trondheim, Norway
thuat.trinh@ntnu.no

Carbon dioxide (CO_2) has an important impact on the climate and is therefore widely studied. Huge efforts are being made, for instance to reduce emissions of CO_2 to the atmosphere, by capture- and sequestration techniques. In that context, carbon membrane is a promising and cheap material to capture CO_2. Knowledge of heat and mass transport of the gas in a graphitic material is essential to design a new class of material. Boundary driven non-equilibrium molecular dynamics is a reliable technique to obtain thermal conductivity of CO_2 in a wide range of temperature and pressure [Trinh *et al.* J. Chem. Phys. 141, 134504 (2014)]. Recently we found that there are two layers of CO_2 adsorbed on a graphite surface [Trinh *et al.* Chem. Phys. Lett. 612, 214 (2014)]. These layers can be considered as distinct thermodynamic systems and are in equilibrium between each other. In this work, we will discuss the transport of heat and mass of CO_2 in a carbon membrane under a temperature gradient parallel to the surface of the pore. By non-equilibrium molecular dynamics simulations, we will show that the pore size and the number of adsorbed layer have an important effect on the transport properties. This will add to the basic understanding of thermal diffusion of CO_2 gas in carbon material.