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Analytical diffusion mechanism (ADiM) model combining specular, Knudsen and surface diffusion

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Abstract

We present a unified transport model that combines specular, Knudsen and surface diffusion mechanisms, termed the Analytical Diffusion Mechanism (ADiM) model. The ADiM model uniquely describes the transport behaviour of the bulk gas and adsorbed phase taking place in rough and smooth nanopores. Experiments and molecular simulations of nitrogen flow through aligned nanotube-based membranes are used to verify the model. In addition, we explore entrance effects using a suction energy mechanism that is compatible with ADiM and can accelerate gas permeance by an order of magnitude. Finally, ADiM is used to assess the effect of tube size on post-combustion carbon dioxide separation from fossil fuel plants.

keywords: diffusion, nanotube, membrane, pore, separation

1 Introduction

Ever since ultra-fast gas transport was simulated in carbon nanotubes (CNTs) [1], experimental efforts have endeavoured to create a system that operates like the Maxwell's demon concept [2],