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

Aaron W. Thornton^{*†}, Afsana Ahmed^{‡‡}, Sridhar Kumar Kannam[□], B. D. Todd[‡], Mainak Majumder^Δ and Anita J. Hill[◇]

[†] CSIRO Manufacturing Flagship, New Horizons, Clayton Campus, Monash University, Victoria 3800, Australia

[‡] Department of Mathematics, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Melbourne, Victoria 3122, Australia

[□] IBM Research Collaboratory for Life Sciences-Melbourne, Victorian Life Sciences Computation Initiative, The University of Melbourne, Victoria 3010, Australia

^Δ Nanoscale Science and Engineering Laboratories (NSEL), Department of Mechanical Engineering, Monash University, Clayton VIC Australia 3168

[◇] CSIRO Group Executive, Private Bag 10, Clayton South MDC, Victoria 3169, Australia

* Corresponding author: Aaron W. Thornton, aaron.thornton@csiro.au, telephone +61 3 9545 8018, fax +61 3 9545 2837

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],

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