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Editorial

Special Issue on "Transport of Fluids in Nanoporous Materials"

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Understanding the transport behavior of fluid molecules in confined spaces is central to the design of innovative processes involving porous materials and is indispensable to the correlation of process behavior with the material structure and properties typically used for structural characterizations such as pore dimension, surface texture, and tortuosity. The interest in fluid transport in nanopores dates back a century, when Martin Knudsen [1] performed experiments on gaseous transport in macroporous glass tubes several microns in diameter and derived the well-known Knudsen diffusion equation for the transport of rarefied gases. Since then, the Knudsen model has been widely used to predict gas transport coefficients in confined spaces and has had a significant impact on technological developments. The Knudsen model was improved by Smolouchowski [2], who showed that the mode of scattering from a solid surface can radically modify flux rates. Subsequently, it was recognized that the Knudsen model suffers from a significant weakness, especially in channels of nanoscale cross sections, because the potential energy field arising from fluid–solid interactions distorts the linear trajectories assumed in classical gas kinetic theory. As a result, this model and others such as the Dusty Gas model [3], which is applicable to dense gas systems, fail at the nanoscale where the impact of fluid–solid interactions is dominant. Moreover, in dense fluids at the nanoscale, it has become clear that that these interactions mean that fluid density is not uniform, which implies that there must be a spatial dependence in viscosity. The recognition that transport in nanoporous materials differs in many respects from macroscale transport has spawned new research in the last decade, particularly to facilitate the development of new technologies at the nanoscale with enhanced efficiency.

The selective nature of transport in nanoporous materials has resulted in numerous new separation processes that have replaced energetically less efficient conventional technologies. Zeolite-and carbon-based membranes have been used to purify azeotropic and saline solutions, for which membrane-based pervaporation and desalination techniques have been developed, exploiting the large surface area and adsorptive capacity of nanoporous materials. Pervaporation involves hydrophilic/hydrophobic surfaces and a phase-change in a liquid, whilst in desalination, as well as in any phase change, the hydration interaction of ions with water molecules plays a central role in determining the rejection ratio. In these and all separations in general, fluid–solid interactions strongly influence adsorption capacity and permeability and therefore the process efficiency. The transport coefficients associated with such systems can be estimated from the analysis of the trajectories of fluid molecules from computer simulations; however, structural non-idealities, lack of reliable models for the solid-fluid interactions, and unduly large computational requirements impose limitations in actual practice. Consequently, the wide variety of structural complexities and interaction forces make

it necessary to combine experiments on permeation and transport with adsorption isotherms and molecular dynamics simulations in order to probe the movement of fluids/ions in confined systems under realistic conditions.

This Special Issue on "Transport of Fluids in Nanoporous Materials" of *Processes* collects the recent work of leading researchers in a single forum, and the contents cover a variety of theoretical studies and experimental applications, focusing on the transport of fluids in nanoporous materials. Despite the interdisciplinary nature of the different applications involved, there is a common characteristic of fluid/ion transport in nanopores connecting the areas together which we seek to capture in this issue. We believe that the advances described by the contributors have significantly helped accomplish this target. Besides the research articles, the issue features a number of reviews, covering a range of topics, which highlight the versatility of the area. For instance, Kärger et al. [4] discuss the direct measurement of transport coefficients for guest fluid molecules in complex nanoporous materials where the signal produced by the H atom is employed to predict diffusivity. Since many fluid molecules contain hydrogen, this approach is very versatile. As an attractive technique, molecular dynamics modeling has the ability to access spatial and temporal resolutions that are difficult to attain in experimental studies. Murad et al. [5] review molecular dynamics techniques to examine intramembrane transport in reverse osmosis (RO), ion exchange, and gas separation. It is comprehensively demonstrated how molecular dynamics simulations provide deep insight into the physiochemical behavior of many such membrane-based applications and aid in more efficient process design and optimization. The review article of Daivis and Todd [6] analyzes the failure of traditional Navier–Stokes theory when applied to transport at the molecular scale in nanofluidics where several fundamental phenomena such as slip, spin-angular momentum coupling, non-local response, and density inhomogeneity require consideration. Theories accounting for these effects are provided and are discussed to improve the accuracy of nanoscale transport modelling. The review of Monsalve-Bravo and Bhatia [7] focuses on models for mixed matrix membranes, an emerging nanomaterial now widely being investigated for gas separations. Such membranes combine the favorable selectivity properties of polymers with high flux capabilities of zeolites or other adsorbents to achieve high separation efficiency, and their modelling is critical to membrane design and optimization. At a more applied level, the review of Zhu and coworkers [8] discusses the synthesis and potential applications of superparamagnetic Nano-Fe_3O_4, an important nanoscale material with desirable properties that are conducive to its application in a number of areas including magnetic resonance imaging, biosensors, and drug delivery. In another application-focused review, Nguyen and Lee [9] discuss the separation of lithium, an important material for battery electrodes, ceramic glass, alloys, dying, and a host of other applications.

Adsorption and separation is one of the key application areas of nanoporous materials where they provide enhanced efficiency, and several articles address problems related to such applications. Gu and coworkers [10] describe experimental measurements of ethanol dehydration by cation-treated zeolite membranes, in which the pore channels were decorated by ion-exchange. The treated membranes achieved the desired pore size, cation charges, and hydrophilicity, thereby significantly enhancing the separation factor. Pore size distribution measurement is an important issue in nanoporous materials and becomes challenging when the pores are in the ultra-microporous range. Ji et al. [11] describe a novel method for determining such pore size distributions based on the measurement of transport parameters and interpreting these through effective medium theory while using a molecular level theory for single pore transport. Qing Liu and coworkers [12] discuss the synthesis of carbon aerogels for CO_2 capture, an application now considered one of the significant challenges of our time. In other adsorption related work, Xue, Ju, and coworkers [13] discuss the synthesis of ion sieves for Li ion adsorption, while Liang, Zou, and Li [14] report the effect of different cyclic stress paths on the damage and permeability changes in gas bearing coal seams. These are all issues of importance to technologies related to our energy future. Of course, there are a host of other areas where nanoscale materials play a role, and some examples are discussed in several important contributions. Liu, Ba, and coworkers [15] applied microfluidics theory to microdroplet dosing for cell culture on a chip to

meet the demand for narrow diffusion distances, controllable pulse dosing, and to lessen the impact to cells. The established mathematical model could analyze the rhodamine mass fraction distribution, pressure field, and velocity field around the microdroplet and cell surfaces. Good accuracy and controllability of the cell dosing pulse time and maximum drug mass fraction on cell surfaces is achieved, and the drug effect on cells analyzed with more precision, especially for neuronal cell dosing. Ye and coworkers [16] discuss a new porous-medium-based burner, which can achieve high energy efficiency, and present its numerical simulation. Combustion in porous media is a subject of long-term interest and continues to attract attention because of its potential for reducing emissions and improving combustion efficiency of low-grade combustible pollutants. Finally, Liu and Zhang [17] present an application for carbon nanotubes as a dispersant in foamed concrete to improve its mechanical properties.

The above papers demonstrate the versatility and technical importance of the area of fluid transport in nanoporous materials, ranging from the formulation of fundamental theory to practical applications. Although the basic principles of fluid transport in the nanoscale are fairly well understood, the articles address outstanding challenges related to fluid transport in different areas in terms of both application and theoretical perspectives, and much remains to be explored in the future. With the enormous variety and number of the applications currently under development, we feel confident for the longevity and future of this subject.

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Guest Editors

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