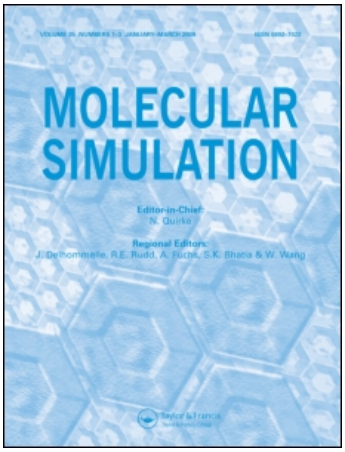

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Guest editorial

Suresh K. Bhatia[a]
[a] Department of Chemical Engineering, University of Queensland, Brisbane, Australia

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Guest editorial

Fluids in confinement display a complex and rich variety of behaviour that is currently being explored extensively and which has profound technological consequences. Such fluids, especially those in nanoscale confinements that are of the order of molecular dimensions, have properties that are remarkably different from their bulk counterparts, and this influences their equilibrium, transport as well as reaction behaviour. While the subject is more than a century old, until recently there was only modest emphasis on the fundamental understanding of confined fluid behaviour. However, the last two decades have seen a major resurgence of interest because of the rapid growth in the applications of new nanomaterials, and the emergence of a vast array of nanotechnologies that exploit the complex behaviour of a fluid in confinement. These applications span a battery of conventional as well as developing technologies pertaining to catalysis, adsorption and separation including membrane-based processes, gas storage, nanolubrication, biochemical lab-on-the-chip systems, micro-electromechanical devices and drug delivery, to name only a few.

It is now well understood that the fundamental assumptions behind the conventional continuum modelling become questionable at the nanoscale, where the atomic-scale texture of the fluid and of the confining surface plays an increasingly important role. A striking example of this is the rapid transport in carbon nanotubes, which is attributable to their relatively smooth energy landscape, when compared with zeolites or other conventional nanoporous materials; or the role of the surface protein structure and charges in mediating transport and switching properties of biological ion channels. Confinement at the nanoscale also leads to inhomogenieties and the breakdown of the usual constitutive laws governing continuum analysis. Statistical mechanics, incorporating appropriate intermolecular interactions, forms the crux of our craft in dealing with these complexities; however, rigorous analytical theories based on mechanical models involving many-body interactions fast become intractable when moving beyond the very simplest of systems. Molecular simulation then becomes the technique of choice in tackling the enormous variety of problems encountered in relation to confined fluid behaviour in applications of the kind indicated above.

This special issue of the journal brings together leading researchers in the area in a single forum, covering a variety of applications where the focus is on confined fluid behaviour. Despite the multidisciplinary nature of the subject and the wide range of systems involved, there is a common thread of molecular mechanics which binds the area and which we seek to capture in this issue. I believe the breadth and the variety of the contributions have helped greatly in achieving this goal. For example, papers from the groups of MacElroy and Baumgaertner discuss the complex issues related to water and ionic transport in carbon nanotubes, which have special relevance to ion channels and other biological systems. Systems involving water have also long been of interest in adsorption science because of the intriguing issues related to hydrogen bonding, wetting and electrostatic interactions with surface functional groups; in recent years, this interest has been enhanced because of their influence on the transport in nanofluidic devices. These issues are addressed in the works from the groups of Fuchs and Aluru, while the paper by Suman and Kumar discusses the role of hydrophobic interactions in dendrimer adsorption on solid surfaces.

The rapid pace of development of new nanomaterials during the last two decades has sparked a parallel effort addressing the challenge in understanding their fascinating adsorption and transport properties. The contributions from several groups (Broadbelt and Snurr; Johnson; Sholl; Papadopoulos and Theodorou; Keil; Srebnik and Sheintuch) provide an important insight into the complex issues pertinent to adsorption and transport in metal organic framework materials, pore mouth modified and pristine zeolites as well as carbon nanotubes and related composite materials. In my own laboratory at The University of Queensland, there has been a sustained recent effort in developing tractable analytical theories of transport in idealised nanopore models for MCM-41 and related silica materials as well as in carbons, in conjunction with simulations; and Nicholson provides a lucid summary of the key results and theories. For carbons, the venerable slit pore has for long been considered a useful idealisation, and the characterisation using the

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Dubinin approach is examined in detail with the help of simulation by Do and coworkers. Sorption related strain has been a topic attracting interest in the recent literature, and its influence on condensation in slit nanopores is discussed in the contribution from Martin Schoen and his group. The levitation of sorbates in narrow pores of the size at which a transition from a single to a double potential well occurs, and its consequences of diffusion, is a phenomenon of importance for zeolites, carbon nanotubes and other adsorbents. The contribution from Krishna and Yashonath shows that a somewhat similar concept also applies to diffusion in solids. Quantum effects on adsorption and transport of hydrogen and its isotopes have also been a subject of recent activity in my group, and the paper by Yang Wang discusses the equilibrium selectivities and optimum conditions for H_2/D_2 mixture separation in slit pore geometry. Reaction in confined systems is another fascinating topic, and as yet there has not been sufficient understanding of the effect of confinement on reaction equilibrium and kinetics. The contribution from Searles and collaborators discusses confinement effects on *n*-butane isomerisation in slit pore geometry, showing that the rate of the *gauche–gauche* transition via the *trans* well is enhanced relative to the *gauche–trans* and *trans–gauche* interconversions. Finally, the contribution from Todd discusses the effect of confinement on chemical wavefronts, showing a reduction in the wavefront speed in sufficiently narrow nanochannels. These works suggest the potential of tailoring the confinement to achieve selective conversion in homogeneous as well as surface catalysed reactions, and the subject will no doubt see increased activity.

The above papers provide a glimpse into the fecundity of the area of confined fluids, both in terms of scientific issues that require our attention and the variety of applications it contacts. At the same time, the articles highlight the commonality in fundamentals underpinning the various topics, which suggests that there is much scope for consolidation and building of the area of confined fluids as a subject in its own right. With the enormous variety and number of the problems being uncovered, I remain optimistic about the longevity and future of the subject.

I thank all the contributors and the Editor-in-Chief, Nick Quirke, for their enthusiastic support of this special issue, as well as the editorial staff of *Molecular Simulation* for their efforts.

Suresh K. Bhatia
Department of Chemical Engineering,
University of Queensland, Brisbane,
Australia