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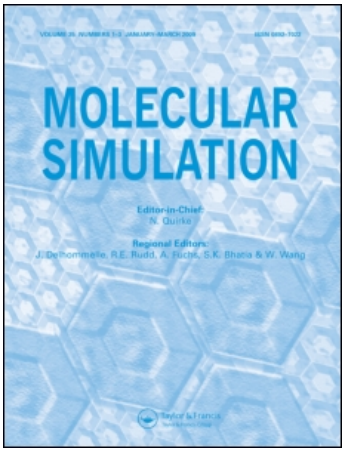

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Editorial

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To cite this Article Haile, J. M.(1989) 'Editorial', Molecular Simulation, 2: 1, 1 — 2
To link to this Article: DOI: 10.1080/08927028908032779
URL: http://dx.doi.org/10.1080/08927028908032779

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Molecular Simulation, 1989, Vol. 2, pp. 1–2
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Printed in Great Britain

EDITORIAL

Chemical engineering can be defined as the amalgamation of chemistry, physics, and mathematics that ultimately results in economic design and operation of processes for producing materials in bulk, as intermediates, and as finished products. It is becoming increasingly clear that forces from both science and the marketplace are driving chemical engineering research to seek molecular explanations for bulk-material behavior; consequently, molecular simulation has become a new tool for those chemical engineers who crave an understanding of phenomena. Understanding is the foundation for successful prediction, which in turn is the foundation for appropriate design and performance.

In November 1987 the annual meeting of the American Institute of Chemical Engineers was held in New York City. A part of that meeting was a one-day symposium on "Molecular-Based Computer Simulations," organized by Professors Pablo Debenedetti and Katherine Shing. A selection of papers presented at the symposium forms this issue of *Molecular Simulation*.

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These papers are representative of the kinds of questions that chemical engineers are asking of molecular simulation. In the chemical engineering community, simulation has been largely devoted to probing thermodynamic properties of fluids and the papers by Dodd and Sandler, Debenedetti, Nouacer and Shing, Randelman *et al.*, and Strauch and Cummings are typical. More particularly chemical engineers need guidance on the behavior of mixtures, so that, although the papers here by Dodd and Sandler, Randelman *et al.*, and Strauch and Cummings are concerned with pure fluids, it is evident that the intent of these papers is to set the stage for future work on mixtures.

In addition, there is now in chemical engineering a healthy expansion of uses of molecular simulation away from fluid phase thermodynamics. New attacks are being made on transport phenomena, such as the paper here by TeGrotenhuis *et al.* on self-diffusion in colloidal suspensions. Moreover, new work is being done on materials in other than purely fluid phases, such as that by Park and MacElroy on bicontinuous random media. It is safe to say that this movement away from fluid thermodynamics will continue.

Aside from these areas, however, are other research areas, missing from this selection, that should see chemical engineering participation in the future. One such area is simulation of biological molecules and processes, which is becoming important in drug design and more generally in the health industry. Another area is molecular simulation of numerous transport phenomena; specifically, one may now perform extensive and realistic molecular dynamics simulations that test, in direct ways, the multitude of assumptions inherent in the continuum mechanical description of transport. Yet another missing area is the simulation of chemical reactions. These areas are not represented here simply because chemical engineers have not yet made efforts to apply simulation to those problems. This neglect will be rectified in the next few years.

Perhaps a general lesson offered by this issue is that the boundaries between science and engineering research are eroding. The questions being asked by science and by engineering, if not always the same are at least very similar; nevertheless, the motivations for those questions are, and are likely to remain, different. Molecular simulation seems to be able to serve as a vehicle by which scientists and engineers can communicate and collaborate in fruitful and mutually beneficial ways.

J.M. Haile

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