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Preface

No one can dispute the central role of transport phenomena in chemical engineering. It is a subject that is of great interest for industrial practice and one that occupies a prominent place in the chemical engineering curriculum. While the macroscopic engineering science of this field is well developed, we are missing for many important systems constitutive relations and means of estimating the transport coefficients that appear in the macroscopic description. Kinetic theory of gases provides simple expressions for the transport coefficients in the dilute gas phase, but similar expressions have eluded researchers for more complicated physical systems. In many areas of current research in the transport field, it is clear that further advances will only come with increased knowledge of how the microscopic properties of a system are related to the macroscopic transport properties. This need exists for bulk systems, but becomes even more evident when considering applications where molecules occupy spaces that are themselves of molecular dimensions. Such applications include heterogeneous catalysis, adsorption separations, membranes, and lubrication. Molecular modeling, in conjunction with experiment and other theoretical tools, is poised to play an important role in developing our understanding of transport phenomena in such systems.

This issue of the *Chemical Engineering Journal* is devoted to ''Molecular Modeling of Transport Phenomena'' in recognition of the role that cutting-edge molecular simulation tools are playing in the traditional chemical engineering field of transport. Molecular simulation has experienced tremendous growth in recent years due to increases in computational power and advances in the simulation algorithms. Such simulations are based on the principles of statistical mechanics and an understanding of the potential-energy interactions between species at the molecular level. The potential energy can be calculated from so-called force field expressions that describe contributions such as dispersion, repulsion, electrostatic, bond-bending, bond-stretching, and torsional energies. Extending the hierarchy of calculations to even smaller scales, the energetics can be elucidated from quantum mechanical calculations.

The papers in this issue are grouped according to topic. The largest group of papers all deal with adsorption and diffusion – on solid surfaces, in microporous materials, or in bulk solids. Transport through membranes is the subject of two papers, and the final three papers focus on transport, structural, and rheological properties of chain molecules at interfaces and in the bulk. These papers provide just a sampling of current research around the world in applying molecular simulation to solve problems in transport phenomena.

It has been a pleasure to compile this issue. I would like to thank Prof. Harold Kung for suggesting a special issue on molecular modeling and for his guidance in preparing the issue. My thanks also to Prof. Richard Darton and Jennet Batten from the journal editorial office. Most of all I thank the authors and reviewers of the 13 papers published here for their fine manuscripts, for their insightful reviews, and for submitting things on time, often under tight deadlines.

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