The Evolution of Molecular Modeling into a Chemical Engineering Tool

The three Commentaries that appear in this issue evolved from communications with Professor J. Richard Elliott of the University of Akron as he was helping organize technical sessions for the Annual Meeting of the American Institute of Chemical Engineers held in Philadelphia in November 2008. This meeting celebrated the 100 Year Anniversary of the AIChE in the city of its origin. These Commentaries originated from two special centennial sessions entitled "The Evolution of Molecular Modeling Into a Chemical Engineering Tool" with presentations by Ilja Siepmann, Anne Chaka, Peter Cummings, Juan De Pablo, David Rigby, and the authors of these three articles. In addition to their own viewpoints, the authors of these Commentaries have included many of those from the other presentations in these sessions.

These Commentaries represent perspectives on molecular simulation and its role in chemical engineering as well as the roles of chemical engineers in developing molecular simulation. Keith Gubbins provides an overview of the history of molecular simulation with an emphasis on its impacts in laying the foundations of model equations and phenomenology. Doros Theodorou focuses on the roles of Monte Carlo simulation as a tool for phase equilibria and for estimating long time behavior when detailed dynamics cannot feasibly approach the fully equilibrated behavior. Maginn and Elliott focus on the roles of molecular dynamics simulation, emphasizing the perpetual pursuit of valid molecular trajectories with finite computational resources.

In all cases, these Commentaries emphasize molecular simulation tools that are available in the present as well as prospects for the future. Applications of the present include equations of state, phase equilibrium predictions, and physical property predictions. Applications under development include mesoscale models, self-assembly, and transition state theory. Molecular simulation is being applied to research fields in biology, nanotechnology, energy, and the environment.

Chemists and chemical engineers have always worked at the nanoscopic level of atoms and molecules. The characterization of molecular interactions at every length scale has been a constant pursuit, from group contribution methods to quantum mechanics. The present status provides reasonable approximations at the atomic scale and the framework for further refinements. These characterizations are informed by data from quantum mechanical computations as well as data from traditional physical property measurements. Even at the present, molecular simulations can provide accuracy for practical applications that supersedes that of previous tools. As refinements advance, broader ranges of properties will be incorporated with greater precision into a unified framework.

I trust that many of our readers will find these Commentaries of interest. I would like to thank all the authors for their efforts but especially Richard Elliott for facilitating these articles for publication here.

Donald R. Paul, Editor

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