Amgen Seminar Series in Chemical Engineering

in

Cherry Auditorium, Kirk Hall, 1 PM

Presents on April 17, 2008

Mainstreaming Molecular Simulation in Chemical Engineering Education and Application

J. Richard Elliott
Dept. of Chemical and Biomolecular Engineering
The University of Akron
Akron, OH 44325-3906

Molecular simulation has made rapid progress in recent years, especially as a research tool. For example, recent results from the Industrial Fluid Properties Simulation Collaborative (IFPSC) have shown that simulation results can rival experimental measurements in accuracy, exposing flawed data and extending limited data. Demonstrations of fundamental phenomenology abound, promising future applications to self assembly, amyloid aggregation, entanglement, and transition states. These developments suggest that molecular simulation is poised to supplant engineering methods like group contributions and corresponding states for engineering properties, at the least. More broadly, future chemical engineers may design molecular structures in the same way that civil engineers design bridges now.

Incorporating this rapid change into the classroom may seem daunting. The curriculum is already crowded. On the other hand, technology is changing the mode of presentation as well as its substance. ConcepTesting permits rapid introduction and assessment of qualitative concepts. Testing can take place in a computational laboratory. These observations suggest a trend with less emphasis on tedious hand calculations while placing greater emphasis on fundamental derivations and conceptual reasoning.

This presentation reviews these developments and describes practical ways of implementing them in the undergraduate classroom. A particular emphasis is placed on discontinuous molecular dynamics (DMD) and the Step Potential Equilibria And Discontinuous Molecular Dynamics (SPEADMD) model for molecular modeling of thermodynamic and transport properties. It is based on DMD and second order Thermodynamic Perturbation Theory (TPT). DMD simulation is applied to the repulsive part of the potential, complete with molecular details like bond angles, branching, and rings. The thermodynamic effects of disperse attractions and hydrogen bonding are treated by TPT. This approach accelerates the molecular simulations in general and the parameterization of the transferable potentials in particular.

One challenge to molecular modeling for process and product design is achieving the connection between nano-scale interactions and dynamics and the macroscale process and material properties. We demonstrate how this connection can be achieved with a chemical process simulator, vapor pressure being a key property. The DMD perspective also dovetails efficiently with the educational initiative of incorporating molecular simulation into the undergraduate classroom. DMD is essentially “billiard ball” physics. Students are familiar with the equations from standard courses in physics. The etomica website makes it possible to visualize the results of this model with virtually no training. Calculating a few collisions eliminates the aura of a black box. Then students can explore the implications of automated computations for large systems over long periods. This perspective can be further enhanced and revisited with conceptual questions focused on the square well potential. Assessment shows that conceptual reasoning is enhanced, even while maintaining traditional student skills in estimating practical properties like relative volatility and coefficient of performance.

This series is at the University of Rhode Island is made possible through the generosity of Amgen, West Greenwich, R.I.