

The Industrial Fluid Properties Simulation Challenge: Highlights of the First Event and a Preview of the Second

J.D. Olson^{C,S}

*The Dow Chemical Company
Research and Development Department
3200 Kanawha Turnpike, P. O. Box 8361
South Charleston, WV 25303, U.S.A.*

For the Industrial Fluid Properties Simulation Challenge Organizing Committee: Ray Mountain¹, Fiona Case², Anne Chaka¹, Daniel Friend³, Jonathan Moore⁴, Dave Frurip⁴, Russell Johnson¹, Joseph Golab⁵, Martin Schiller⁶, and Petr Kolar⁷

This poster describes the results, activities, and philosophy of the Industrial Fluid Properties Simulation Challenge (<http://www.cstl.nist.gov/FluidSimulationChallenge/>). The goal of the Industrial Fluid Properties Simulation Challenge is to obtain an assessment of current abilities and boundaries in the prediction of physical properties for fluids with industrial relevance. This competition is a recurring event to drive improvements in the practice of molecular simulation, formalize methods for the evaluation and validation of simulation results with experimental data, and promote relevance of simulation activities to industrial needs.

The first competition (2001-2002) challenged practitioners of molecular simulation to calculate accurate physical properties for pure materials and mixtures at specific state points. The chosen properties were vapor-liquid equilibria, density, and viscosity. With ten entries to the three problems, the contest ended with the announcement of the Champions at the 2002 Annual Meeting of the AIChE (November 3-8, 2002). Cash prizes were awarded from contributions by BP and The Dow Chemical Company. The Computational Molecular Science and Engineering Forum (CoMSEF) of the AIChE sponsored the contest and NIST administered the event.

Details on the second contest, which is scheduled to begin in September 2003 and end in November 2004, will be presented. The three problem areas for the second contest have tentatively been chosen as: vapor pressure and heat of vaporization, gas solubility (Henry's Law constants), and heat of mixing. A short review of quantitative prediction of phase equilibria and thermophysical properties by molecular simulation will also be presented.

¹NIST, Gaithersburg, MD; ²Colgate-Palmolive Company, Piscataway, NJ; ³NIST, Boulder, CO; ⁴The Dow Chemical Co., Midland, MI; ⁵BP, Naperville, IL; ⁶E.I. du Pont de Nemours & Co., Inc., Wilmington, DE; ⁷Mitsubishi Chemical Corporation, Okayama, Japan.