

The First Industrial Fluids Properties Simulation Challenge

<http://www.cstl.nist.gov/FluidSimulationChallenge/>

Accurate physical property data is critical in process design, but it can be challenging to obtain reliable information, especially for unusual materials, mixtures, or state points far from ambient conditions. Some data are available in the literature, or can be estimated using empirical correlations based on literature data. Resources exist to aid the experimental evaluation of data at NIST, in the AIChE DIPPR consortium, and at a diminishing number of contract measurement laboratories. **But computer simulation holds out great promise in this area.** In the future we would hope to build models of sufficient accuracy to confidently predict physical properties, even for materials that had never been studied experimentally. The AIChE meeting in Indianapolis marked the culmination of the “**First Industrial Fluids Properties Simulation Challenge**” established by a number of industrial companies, and sponsored by the AIChE CoMSEF division, to judge the progress of the computer simulation community towards this lofty goal. The open challenge made at last year's meeting, was to predict densities, viscosities, and vapor liquid equilibria for a specified set of industrially relevant organic fluids and mixtures. For comparison, these properties were also evaluated experimentally by teams at Dow Chemical and NIST. At a well attended session on Sunday the “Great Lake Regressors”, a team of researchers from the University of Minnesota, University of Notre Dame, Wayne State University, and SUNY Buffalo, were recognized as the only group able to attempt to prediction of both equilibrium and transport properties using the same approach, and their success in predicting vapor liquid equilibria for mixed systems without fitting to experimental data for the pure components. The champion in the density prediction section was Huai Sun from Aeon Technology in San Diego. **The champions in the viscosity prediction for n-nonane/isopropanol mixtures were [Marcus Martin](#) and [Aidan Thompson](#) from Sandia**, and the most accurate prediction of vapor liquid equilibria for mixtures of dimethyl ether/propylene and of nitroethane/propylene glycol was obtained by Andreas Klamt from COSMOlogic GmbH. The organizing committee felt that the competition was successful in providing an assessment of current capabilities, and promoting the development of industrially relevant simulation techniques they plan to repeat the challenge, with different properties and materials, in 2003-2004.

First Industrial Fluid Properties Simulation Challenge Committee:

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