Second Industrial Fluid Properties Simulation Challenge

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The Industrial Fluid Properties Simulation Challenge is an opportunity for the molecular simulation community to predict fluid properties that are not available in the open literature. This competition is an open, biannual program that is sponsored by the Computational Molecular Science and Engineering Forum (CoMSEF) of the American Institute of Chemical Engineers (AIChE) and by the Theoretical Subdivision of the American Chemical Society (ACS) Physical Chemistry Division.

NIST in collaboration with scientists at Dow, BP Amoco, Case, Mitsubishi Chemical, 3M, and DuPont have organized the Second Industrial Fluid Properties Simulation Challenge.

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The goal of the Second Industrial Fluid Properties Simulation Challenge was to evaluate and benchmark the available molecular simulation methods and force fields on problems that have significant industrial relevance. This process will encourage the continued development of better algorithms, methods, and force fields, while improving the alignment of academic efforts with industrial needs. Molecular simulation has been identified as a promising technology for predicting thermophysical properties in the Vision 2020 Roadmap for the Chemical Industry. The industrial participation within the organizing committee was even stronger than for the first challenge, and the financial contributions from this sector, which were applied largely for prizes for the most successful entrants, were substantial. Further, the number and quality of the entries submitted to the challenge indicated an increased interest in the process, and the contest has attained a truly international stature, with entrants, judges, and organizers from around the globe.

The three problems in the challenge were announced at the 2003 Fall ACS meeting. Entrants had one calendar year to complete their projects. Benchmark values and uncertainties for the specific problems presented were determined by scientists at NIST and Dow Chemicals, through a combination of new experiments and extensive evaluation of available information. These benchmark results were used to evaluate the second challenge entries. There were five entries in problem 1, five entries in problem 2, and two entries in problem 3.

Challenge 2003 was to predict:

- **vapor pressure and heat of vaporization (problem 1)**
- **Henry's law constants (problem 2)**
- **heats of mixing for specific materials and conditions (problem 3)**

The entries were evaluated in a two-step, double blind process. In the first step, experts in the area of molecular simulation, who were not associated with the organizers and were not entrants, evaluated the overall scientific quality of the entries. Then the entries were ranked by the organizing committee in terms of how accurately the simulation based predictions of fluid properties reproduced the experimental values. The experimental values were not available in the open literature so the entries were predictions.

The results of the competition were announced at a special session of the National Meeting of the AIChE in November 2004. For some of the problems, the entrants were able to produce reasonable predictions for the unknowns, at a level nearly adequate for some industrial purposes. However, for the most challenging problems, especially heats of mixing of the assigned aqueous system, considerable work will be needed before the technique will produce reliable results.

More information is found on the website at http://www.cstl.nist.gov/FluidSimulationChallenge/