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Announcement

SECOND INDUSTRIAL FLUID PROPERTIES SIMULATION CHALLENGE

The Computational Molecular Science and Engineering Forum (http://www.comsef.aiche.org) of the American Institute of Chemical Engineers (AIChE) and the Physical Chemistry Division of the American Chemical Society have established an open competition for scientists and engineers to use molecular simulation methods for a set of industrially relevant problems. The second competition will focus on prediction of vapor pressures and heats of vaporization, gas solubility, and enthalpies of mixing for materials.

The primary goal of the Industrial Fluid Properties Simulation Challenge is to obtain an in-depth and objective assessment of our current abilities and inabilities to predict thermophysical properties of industrially challenging fluids using computer simulation.

The competition is organized by scientists from 3M, BP, Colgate-Palmolive, Dow Chemical, DuPont, Mitsubishi Chemical, and the National Institute of Standards and Technology.

The competition began September 2003 when the problems were announced. *Entries are due September, 2004.*

Full details are available at http://www.cstl.nist.gov/FluidSimulation Challenge. The challenge is open to researchers from academia, government laboratories, and industry not affiliated with the organizing committee. Participants must register at the web site to ensure that their proposed methodology is eligible. Champions will be announced, and cash prizes awarded, at a special session of the AIChE National Meeting in November, 2004.

Industry is seeking successful methods, based on molecular simulation techniques, for prediction of properties of fluids and mixtures. This challenge is in part geared towards ensuring the relevance of academic

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simulation activities to industrial requirements. Successful participants will have the opportunity to transfer their methods to industry.

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