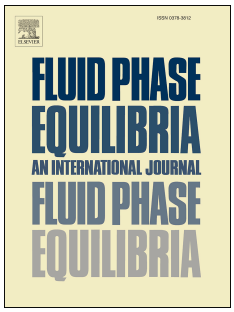

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The Ninth Industrial Fluid Properties Simulation Challenge

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Abstract

The Ninth Industrial Fluid Properties Simulation Challenge aimed to test the ability of molecular modeling approaches to predict water/oil interfacial tension (IFT) at conditions of high temperature and pressure. In particular, the challenge featured water/oil IFT where the oil was n-dodecane, toluene, or a 50:50 n-dodecane/toluene blend at 1.825 MPa and temperatures in the range of 383 K to 443 K. Seven entries were received including approaches such as molecular dynamics (MD) and Monte Carlo (MC) simulations, COSMO-RS, and iSAFT, and they were judged by comparison to pendant drop tensiometer benchmark data. The quality of predictions varied among the entries between approximately 20 % and 70 % of the total points possible with the entries based on MD and MC having the highest scores in most cases. As is often the case in molecular modeling, predictions of the relative trends tended to be reliable even if the absolute values were not.