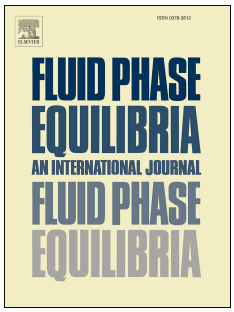

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Predictions of fluidities of amines by molecular simulations: TraPPE-EH vs. OPLS-AA

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ABSTRACT

Amines have several important industrial properties and commercial applications, such as gas sweetening and carbon capture; the synthesis of tranquilizers, decongestants, and azo dyes. For the design of many engineering applications, it is important to calculate the density and viscosity of the substances in order to determine how the fluids should be handled, stored, and discarded. In this work, the accuracy of two common force fields for amines, TraPPE-EH and OPLS-AA, was evaluated with respect to their predictions of liquid densities and fluidities for a large set of amine molecules including primary, secondary and tertiary. We propose the use of the reciprocal of viscosity, the fluidity, as a more accurate assessment of the predictions of viscosity at different