

Viscosity of Simple Fluid Models Using Molecular Dynamics and Application to Petroleum Fluids

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High pressure viscosity is one of the key physical properties for the design of a large number of petroleum facilities. In this work, extensive nonequilibrium molecular dynamics simulations have been performed on Lennard-Jones (LJ), Lennard-Jones Chains (LJC) and isotropic multipolar pure fluids for a wide variety of thermodynamic states. In addition, simulations on mixtures have been carried out in order to question the choice of the combining rules and to assess the limitations of a one-fluid approximation on the molecular parameters. It will be shown that these fluid models, despite their simplicity, are generally sufficient to yield a good estimation of the viscosity of some petroleum fluids under reservoir conditions, such as acid gases mixtures (composed of methane, carbon dioxide and hydrogen sulfide), provided that the density and the temperature are used as inputs and that the fluids are non associative. In addition, using the database obtained by Molecular Dynamics simulations, simple correlations have been constructed to estimate the viscosity of these fluid models. Then, by using a corresponding states scheme and a van der Waals one fluid approximation, it will be shown that these correlations may be used to provide a good estimation of the viscosity of real fluids mixtures with, at most, one parameter per compound adjusted on pure fluid data. The method was extensively tested against available data on multi-component petroleum mixtures and it will be shown that it could be applied on gases as well as on liquid mixtures.