

Modelling the Viscosity of Simple Fluids based on the Enskog-2 σ Model

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There is a clear need for predictive methods for viscosity that are accurate, reliable, internally consistent and, as far as possible, based on a solid theoretical understanding of the underlying molecular interactions. A starting point of a number of such approaches for dense fluids is Enskog's formulation [1], that characterizes molecules by a hard sphere diameter. We have recently developed a new Enskog-2 σ model [2] which is based on Enskog theory and makes use of two effective diameters to represent two aspects of molecular interactions, namely static and dynamic. The model was successfully tested in the supercritical region [2] for a number of simple molecules (Ar, N₂, CH₄ and CO₂). In this work we demonstrate that the Enskog-2 σ model can be extended to predict the viscosity of the fluids at subcritical conditions both in the vapour as well as in the liquid phase, up to very high densities. Modelling the viscosity at high densities requires appropriate corrections to Enskog theory that can be obtained by MD simulations [3]. We make use of MD corrections and present several extensions of the Enskog-2 σ model. The predictions of the model are compared with the available viscosity data and the results indicate the applicability of the model up to high density liquid states. More importantly we demonstrate that the chain like representation of molecules, as successfully used in SAFT [4] and VW [5], is also possible within Enskog-2 σ model. This allows the Enskog-2 σ model to be used to predict the viscosity of n-alkanes. For this purpose we represent each alkane molecule as consisting of m methane like segments. The new chain version of the Enskog-2 σ model is used to predict the viscosity of a number of shorter alkanes (C₂, C₃, C₄) and the resulting deviation plots are presented and discussed.

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