General Friction Theory Model for Thermal Conductivity

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In the area of non-equilibrium properties, the Friction Theory [1] (FT) is an approach that has enjoyed much success for the prediction and modelling of the viscosity of a wide range of fluids. In essence, the friction theory regards a fluid as a stack of layers shifting under a dragging force, as explained in detail elsewhere [1, 2]. The FT uses an equation of state (EoS) as the core of the model, and when the EoS is applicable to mixtures in a thermodynamically consistent manner, such as cubic or SAFT type of EoS, the approach can also be extended to mixtures. Furthermore, the one-parameter FT model [3] has been successfully applied to the viscosity description of an ample spectrum of fluids of industrial applicability and their mixtures – including crude oil. Of relevance to this contribution, it is interesting to observe the physical connection that Müller-Plathe and co-workers have established (though the reverse non-equilibrium molecular dynamics (RNEMD) approach [4–6]) between viscosity and thermal conductivity. When estimated from RNEMD, basically the same non-equilibrium molecular dynamics (MD) technique is applied to the estimation of both viscosity and thermal conductivity. Following this analogy, the FT approach has been further extended to the calculation of thermal conductivity obtaining a similar quality of results as in the case of viscosity (including the correct reproduction of the critical divergence that is consistent with pure fluids and azeotropes). In this work, we explore the development of a general approach for the modelling and prediction of the thermal conductivity of fluids of industrial interest. The objective is a model along the lines of the one-parameter FT viscosity model [3] that has been used for wide industrial applications. Unfortunately, there are not as many experimental data available as for viscosity. This makes it, however, even more important to develop a model that is based on physical insight, so that reasonable results are obtained or predicted even if no reliable experimental data are available.

References:

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