Towards a coarse grained molecular representation valid both for static and transport properties

Guillaume Galliero

Laboratoire des Fluides Complexes et leurs Réservoirs (UMR-5150 with CNRS and TOTAL), Université de Pau et des Pays de l'Adour, BP 1155, F-64013 Pau Cedex, FRANCE

Corresponding author e-mail: guillaume.galliero@univ-pau.fr

1. Introduction

For the time being, there exist two main philosophies to estimate fluid thermophysical (equilibrium, interfacial and transport) properties under typical petroleum reservoir conditions:

- Precise molecular representations combined with extensive molecular simulations (accurate but time consuming, dozens of parameters per species, not widely used in the industry)
- Macroscopic correlations, which are property-dependent and designed for purpose (fast but inadequate when extrapolated to new systems, three to four parameters per species, widely used in the industry)

In this work, we are looking for the best of these worlds and we therefore propose a compromise between these approaches. To do so, we are developing a scheme based on a coarse-grained molecular model that will require a limited number of "microscopic" parameters to describe each species, yet providing accurate description of all "macroscopic" thermophysical properties simultaneously.

2. Towards a coarse grained representation

As an initial coarse grained molecular model we have employed the flexible Lennard-Jones Chain (LJC) model. It has been already largely studied by molecular simulations and accurate equation of states/correlation have been developed to describe its thermophysical properties [1-3]. Furthermore, as this model is fully defined by three "molecular" parameters, a simple link of these parameters with some macroscopic quantities such as critical point location and acentric factor can be established.

As shown in Figure 1, the LJC model is sufficient to provide a reasonable description of the equilibrium properties of some normal-alkanes. Unfortunately, this three parameters model is insufficient to provide accurately the liquid viscosity of long chains at low temperature with the same "molecular" parameters [4].

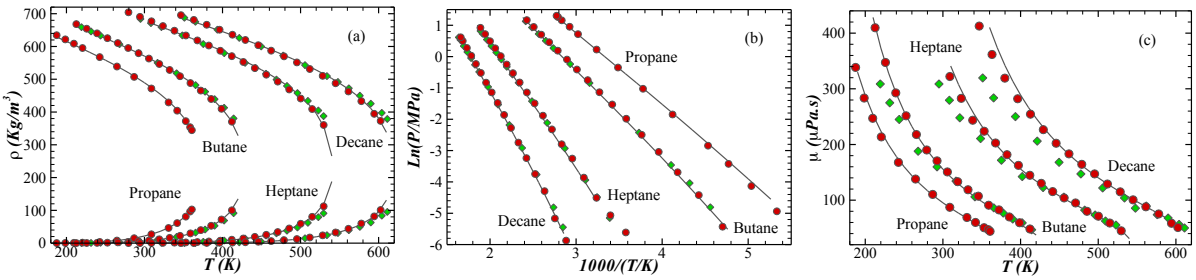

Figure 1: Thermophysical properties of some normal alkanes. a) Vapour-Liquid equilibria, b) saturation pressures c) Liquid viscosities. Lines correspond to experimental data, green diamonds to LJC results and red circles to Mie Chains results.

As we will show during the conference there exist some possibilities to improve these results while keeping a simple coarse grained molecular model (in figure 1 the example of the Mie chain fluid is shown). In addition, we will show that, to ensure the uniqueness of the set of "molecular" parameters associated to the coarse grained model, one has to take into account not only equilibrium properties but also transport properties.

3. Conclusion

In this work a heuristic scheme is proposed to define the simplest coarse grained molecular model able to provide simultaneously equilibrium, interfacial and transport properties of simple fluids. One interest of such an approach is that the so defined coarse grained model can be combined with modern molecular thermodynamics to deduce its fluid thermophysical properties without molecular simulations [5-7].

References

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