Thermophysical Properties of Diesel Fuels at Extreme Pressures: Compositional Analysis, Experimental Measurements and Molecular Dynamics Simulations

Martin Trusler [C, S]
Department of Chemical Engineering, Imperial College London, London, United Kingdom

Linda Naamar, Benoit Creton and Carlos Nieto-Draghi
Thermodynamic and Molecular Simulation Department, Institut Français du Pétrole, Rueil-Malmaison, France

Fausto Ciotta
Department of Chemical Engineering, Imperial College London, London, United Kingdom

Cyril Dartiguelongue
Physics and Analysis Division, Institut Français du Pétrole, Solaize, France

The performance of Diesel engines, measured in terms of emissions and specific consumption, generally improves with increasing fuel-injection pressure. In order to design the next generation of Diesel fuel injection systems, knowledge is required of the thermophysical properties of typical fuels at pressures up to 300 MPa or even higher. The objective of the present project is to validate a methodology for obtaining these properties rapidly from a combination of compositional analysis and modelling approaches. In order to validate this approach, we have used the following strategy:

1. Experimental measurements of viscosity and speed of sound have been made on representative fuel samples at temperatures between (263 and 423) K and pressures up to 400 MPa. The thermodynamic properties of the liquids have been obtained by combining the sound-speed data with measurements of density and isobaric specific heat capacity at ambient pressure.
2. A detailed compositional analysis of the same fuels has been performed by comprehensive two-dimensional gas chromatography (GC×GC). This technique, based on the hyphenation of two capillary columns of different polarities, enables Diesel fuels to be characterized by both chemical family and carbon number, leading in this case to approximately 150 component clusters.
3. These clusters were reduced to typically five pseudo-components by means of an adapted lumping method designed to mimic the bulk physical properties of the initial fuel.
4. Molecular dynamics (MD) simulations (equilibrium and non-equilibrium) were then performed on the simplified mixtures to obtain thermodynamic properties, shear viscosity and rheological behaviour using Anisotropic United Atom (AUA) intermolecular potentials.

The MD results obtained for the simplified mixtures show satisfactory agreement with direct measurements on the original fuels. This will be illustrated by presenting a complete set of results for one particular fuel. The component lumping procedure is tested by comparing experimental measurements on both the original fuel and the simplified mixture.