

Potential Approaches towards the Characterization and Property Estimation of Heavy Petroleum Fluids and Natural Gas Systems

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The optimum design and operation of various units in petroleum production, processing, transportation, and storage depend on the availability of reliable and accurate thermodynamic and physical property data such as viscosity, enthalpy, equilibrium ratios, interfacial tensions, etc. As experimental determinations of these properties under various operating conditions are difficult, if not impossible, time consuming, and expensive, accurate estimation of these properties is becoming increasingly important.

Thermophysical properties are usually estimated through equations of state or generalized correlations which require critical properties and an acentric factor. While these properties are known for light hydrocarbons with carbon numbers up to C₂₀, for heavier hydrocarbons these properties are estimated through available methods. For undefined petroleum fractions, characterization methods are used to estimate these properties from available measurable properties such as distillation data, density, refractive index, composition, or viscosity.

In process simulators, there are some dozen different characterization methods for the estimation of basic properties of petroleum fractions. These methods are based on available data and their extrapolation to heavy hydrocarbons (> C₂₀) lead to differences that could have a significant impact on design calculations, as discussed in a recent ASTM book [1]. Group contribution methods can be applied to pure compounds with the same carbon number as those compounds with known critical constants which were used in their developments. For undefined petroleum fractions, a group contribution method cannot be used, as the structures of the compounds are not known. Furthermore, due to thermal decomposition of heavy hydrocarbons, distillation data for heavy fractions are not available. Thus design calculations for processing of very heavy fractions are based on a use of characterization methods that could lead to serious errors on calculated data for design purposes.

The purpose of this presentation would be to look at the difficulties in characterization of heavy petroleum fractions and standardization of reported critical constants for heavy hydrocarbons. The potential use of directly measurable properties such as velocities of sound or light in the estimation of properties of petroleum fractions through equations of state will be demonstrated. Use of other measurable properties, such as dipole moment, as a potential characterization parameter for heavy hydrocarbons and petroleum fractions will also be discussed in this presentation.

- [1] M.R. Riazi, "Characterization and Properties of Petroleum Fractions," ASTM International, Conshohocken, PA., 2005 [<http://www.astm.org/mnl50.htm>].