Characterization of Complex Hydrocarbon Mixtures via Simulation

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The characterization of heavy oils and bitumen is a fundamental step towards the design, simulation, and optimization of solvent extraction plants and distillation facilities. Recently developed assays such as the ASTM D5236 and Bruno's new distillation assay methodology provide well defined saturated bubble temperatures. These new types of assays lend themselves to fast and rigorous computer simulation of experiments without the ambiguities introduced by earlier assay types such as the ASTM D86 or ASTM D1160 vacuum distillation; no inter-conversion curves are necessary to convert the recent type of assay data into true boiling point (TBP) data. A methodology is presented to determine pseudo-component mole fractions that match the boiling point data from these assays. With pseudo-components defined equation of state interaction parameters are estimated for the modeling of bitumen-solvent mixtures and compared to experimental measurements of solvent content in bitumen at low pressures.