Construction of Digital Oil for Bitumen

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Recovery of bitumen is more complicated and expensive than that of conventional oil due to the extremely high viscosity. For effective production of bitumen, it is required to know oil properties under reservoir and production conditions with various kinds of solvents. In this study, molecular structures of bitumen were investigated in detail to make a molecular model for whole the bitumen compounds, namely “Digital Oil”.

The bitumen sample was first separated into four fractions: saturates, aromatics, resin and asphaltene (SARA), by heptane extraction and column chromatography. They were respectively analysed by elemental analysis, molecular weight measurement using gel permeation chromatography (GPC), ^{1}H-NMR and ^{13}C-NMR to determine hydrogen and carbon types. The carbon aromaticities of SARA are 13, 31, 40 and 48%, respectively. Average molecular weights (g/mol) of SARA are 583, 676, 1131 and 1091, respectively. The molecular weight distributions of resin and asphaltene are broad and asymmetry in comparison with those of saturates and aromatics. Quantitative molecular representative (QMR) method [1], which provides a set of molecules consistent with all the analytical experiments, was used to construct molecular models for each fraction on the basis of molecular “building blocks”. QMR molecular set was improved especially for asphaltenes by adding carboxylic acid building blocks, implying that bitumen might be acid oil. From some trials, average numbers of fused ring units (FU) for SARA were confirmed as 1.3, 1.6, 2.1 and 1.1, and those of aromatic rings in FU are 1.0, 1.8, 3.9 and 6.3, respectively. Since all the fractions are massive, we have further developed our method by generating a number of QMR sets and imitating the molecular weight distributions. Digital Oil was finally constructed by mixing the SARA models for investigation of thermodynamic properties of bitumen with molecular dynamics simulations.

[1] Boek *et al*. (2009) *Energy & Fuels* **23**, 1209-1219.