Comparing Model Asphalt Systems Using Molecular Simulation

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Asphalt is a mixture composed of hundreds of organic compounds. Based on solubility and polarity, asphalt can be divided into three parts: asphaltene, resin, and maltene. Among them, asphaltene is the most viscous and most polar. Maltene is mainly composed of aliphatic molecules and is nonpolar and the least viscous. Resin polarity and viscosity is in between that of asphaltene and maltene.

Two different ternary mixtures were simulated, with a long-term goal of matching properties of Strategic Highway Research Program (SHRP) core asphalts. A different asphaltene molecular structure from the literature was used in each mixture, while dimethylnaphthalene represented resin and n-C_{22} represented maltene.

The density, heat capacity, and modulus of these mixtures were calculated using molecular simulation. Glass transition temperatures of these two mixtures and orientation between molecules were analyzed. One surprising preliminary result is a suggestion that asphaltenes are more commonly perpendicular to each other, rather than parallel.