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Study of Asphaltene Behavior with N6 Structure in Aromatic Solvents by Molecular Dynamics Simulation

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INTRODUCTION

Crude oil is composed of materials such as saturated, aromatic, resin and asphaltenes, and the extraction and utilization of oil reservoirs will depend heavily on the chemical structure and composition of the percentage of crude oil components. Among these materials, asphaltenes play an important role in this field because of their complex nature and cumulative behavior. The effect of asphaltene molecular structure on the sedimentation properties of 8 different types of asphaltene molecules using molecular simulations have been investigated by Sedghi et al [1].. In addition, their results show that the interaction between aromatic carbon-bearing rings π-π in the center of the asphaltene molecule is the main factor in the accumulation of asphaltene molecules. Therefore, in this study, the solubility of asphaltene molecules with N6 structure in solvent solvents such as cyclohexane, toluene, benzene, chlorobenzene and bromobenzene is considered accurately by using molecular dynamics simulation. From analysis of concentration, the radial distribution function (RDF) is used to examine the dissolution mechanism or the accumulation of asphaltene molecules in different solvents as well as the interaction between them.

METHOD AND SIMULATION DETAILS

To perform molecular simulations, steps must be taken to create the molecular structure of the material, construct the simulation box, provide basic information, force fields, select the appropriate simulation method, and interpret

and test the results accordingly. To perform molecular simulations, the molecular structure of all molecules should be determined, drawn and optimized. To this end, the molecular structure of the asphaltenes N6 and all solvent molecules such as cyclohexane (C6H6), toluene (T), benzene (B), chlorobenzene (ClB), and bromonazene (BrB) solvent are optimized and structurally optimized. The molecular mass and the chemical formula of asphaltene molecule N6 structure is 79.49 g/mol and C57H63NS respectively. A review of previous studies in this field suggests that the COMPASS force field be used to model the interactions of asphaltene molecules as well as different solvents, and this force field can predict good equilibrium properties of asphaltene.

RESULTS AND DISCUSSION

The physical properties such as density and the solubility parameter of asphaltene and solvents are calculated to verify the validity of the simulation results. Therefore, the density and solubility parameter of asphaltene N6 and solvents such as cyclohexane (C6H6), toluene (T), benzene (B), chlorobenzene (ClB) and boronbenzene (BrB) by using the molecular dynamics and the ensemble of NPT at ambient temperature and pressure are calculated. The solubility parameter of toluene 18.25 $MPa^{0.5}$ is calculated, which it has a good and acceptable consistency with the data which have been reported by Amjad et al [2], i.e. 18.30 MPa0.5 because the simulation details, method and software used are the same. On the other hand, the simulation densities of cyclohexane, toluene and benzene solvents was 0.77, 0.86, and 0.84 g/cm^3 respectively, with the experimental data of 0.773, 0.862 and 0.873 g/cm^3 are good and acceptable. The lowest and maximum error rates calculated for simulation data were calculated to be 0.23 % and 4.33 % respectively, which the calculated rates indicate the high accuracy of the results.

Therefore, it can be said that the selection of the COMPASS force field and the simulation details for the investigation of the asphaltene molecules in various solvents is quite correct. Also, the comparison between the simulation results and the results presented by Amjd et al suggests that they be very well adapted to each other. In Figure 1, the RDF of asphaltene molecules is plotted before and after the simulation. As the results show, before the simulation of asphaltene molecules are very distant from each other, and they are dispersed within the simulation box, but after the molecular dynamics simulations, the asphaltene N6 molecules approach each other and they are located at the distance of 5.1 Å from each other.

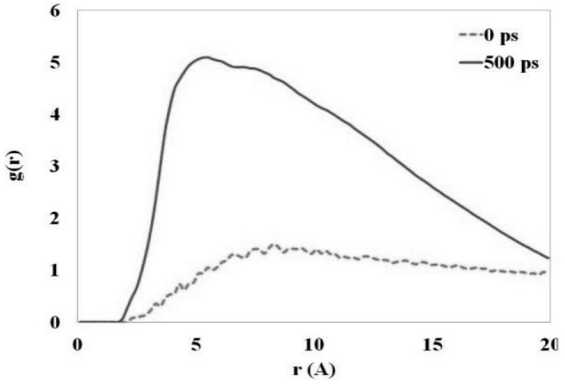

Figure 1: The RDF of the asphaltene molecules.

The behavior of 12 wt.% solution of asphaltenes N6 in the Cyclohexane, toluene, benzene, chlorobenzene and bromobenzene solvents at ambient temperature and pressure is investigated by molecular dynamics method. RDF of asphaltene molecules in different solvents are shown in Figure 2. The results show that the RDF of asphal

tene molecules in a solvent has a sharp peak of 4.5 Å, which indicates the equilibrium distance of the asphaltene molecules in the cyclohexane solvent, and confirms that the asphaltene molecules are aggregating.

Similar to this, in RDF, asphaltene molecules are also found in the benzene solvent, but its intensity is also lower.

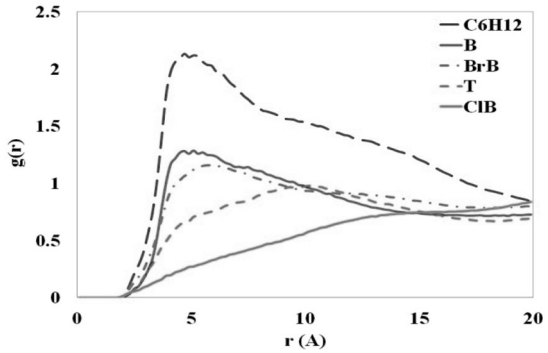

Figure 2: The RDF of the asphaltene molecules in different solvents.

CONCLUSIONS

The results showed that asphaltene molecules, due to the aromatic rings and the π-π interaction, as well as the heteroatoms S and N in their core, tend to accumulate and precipitate, and when they are added aromatic solvents, solvent molecules along with the nucleus of asphaltene molecules prevent their accumulation, and they dissolve solvent in solvent.

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