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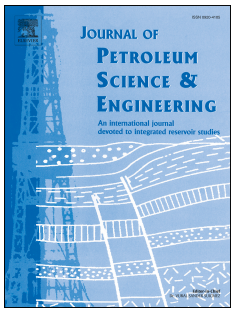


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# Molecular Dynamics Studies of Interaction between Asphaltenes and Solvents

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## Abstract

Understanding of the molecular interaction between asphaltenes and other molecules, which may act as its solvents, provides insights into the nature of its stability in petroleum fluids and its phase transitions. Molecular dynamics simulations were performed and reported here on systems consisting of a single asphaltene molecule and pure solvents. Three types of asphaltenes with different architectures, molecular weights, and heteroatoms content were investigated. Water and ortho-xylene were selected to be the interacting solvents. All simulations were performed by using GROMACS software. OPLS_AA potential model for hydrocarbons and SPC/E potential model for water were used in simulations. It was shown that the polar functional groups in asphaltenes were responsible for generating hydrogen bonds (HBs) between asphaltenes and water. It was also demonstrated that both electrostatic (ES) and van der Waals (vdW) interaction energies between asphaltenes and water had important roles. On the contrary, ES between asphaltenes and ortho-xylene had a minor effect as compared with the vdW. In all cases, potential energies increased rather slightly when the pressure was boosted. Moreover, they decreased noticeably when the temperature was raised. HBs between asphaltenes and water were not influenced by pressure change. Additionally, they increased slightly when the temperature was dropped.

**Keywords:** Asphaltene; molecular dynamics; solvent; ortho-xylene; water; intermolecular potential energy.

### Notations

| | |
|---|---|
| A | Asphaltene |
| COOH | carboxyl group |
| D | Debye |
| E | potential energy |
| ES | Electrostatic |
| GROMACS | GROningen MAchine for Chemical Simulations |
| H | hydrogen |
| HB | hydrogen bond |
| MD | molecular dynamics |
| NH | amine group |