

# Accepted Manuscript

Molecular dynamics studies of interaction between asphaltenes and solvents

Salah Yaseen, G. Ali Mansoori

PII: S0920-4105(17)30491-6

DOI: [10.1016/j.petrol.2017.05.018](https://doi.org/10.1016/j.petrol.2017.05.018)

Reference: PETROL 4002

To appear in: *Journal of Petroleum Science and Engineering*

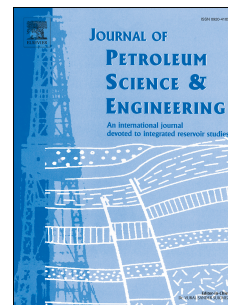
Received Date: 24 February 2017

Revised Date: 10 April 2017

Accepted Date: 17 May 2017

Please cite this article as: Yaseen, S., Mansoori, G.A., Molecular dynamics studies of interaction between asphaltenes and solvents, *Journal of Petroleum Science and Engineering* (2017), doi: 10.1016/j.petrol.2017.05.018.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# Molecular Dynamics Studies of Interaction between Asphaltenes and Solvents

Salah Yaseen <sup>a,\*</sup> and G.Ali Mansoori <sup>b</sup>

<sup>a</sup> Department of Chemical Engineering, University of Illinois at Chicago, Chicago, IL 60607-7052, USA; syasee3@uic.edu

<sup>b</sup> Departments of Bio- and Chemical Engineering, University of Illinois at Chicago, Chicago, IL 60607-7052, USA; mansoori@uic.edu

\* Corresponding author

## 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

Download English Version:

<https://daneshyari.com/en/article/5484093>

Download Persian Version:

<https://daneshyari.com/article/5484093>

[Daneshyari.com](https://daneshyari.com)