DPD study of water-petroleum emulsions in presence of functionalized copolymers

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The world's growing energy demand has boosted the production of more and more heavy and extra-heavy oil that in some cases is contaminated by water in the form of free water or emulsion during the well production. This wastewater must be broken to separate water from oil in order to prevent additional transportation volume and corrosion in the equipments. The removal of this emulsionated water in oil is first driven by a gravity process; however, the reduction of water content in heavy and extra-heavy oils is not a direct process because the stability of water drops with respect to the gravity force in the oil fluid.

The treatment of petroleum wastewater is carried out mainly by mechanical, electric and chemicals methods. From these methods, the most common way of water removing is the use of external alternating current or direct current fields [1-2] which produce the coalescence of the water drops and the breaking of the water-in-oil emulsion. However, the effectiveness of the electric methods decreases when the viscosity and density of the oil are incremented.

In the case of chemical desemulsifiers the variety goes from alcohols, fatty acids, fatty ammines, glycols, alkylphenol products and a large variety of polymers [3-4]. In this work, we focus in the interaction between a functionalized copolymer in an oil-water emulsion in order to discern the stabilized geometric configuration in the oil-water-copolymer emulsion based on Dissipative Particle Dynamics (DPD) [5]. We chose a triblock model for the copolymer structure formed by the sequence:

$(F)(PE)_{10}(PO)_{10}(CEN)_1(PO)_{10}(PE)_{10}(F)$

Where, PE, PO, CEN and F are propylene oxide, ethylene oxide, ethylene glycol and di-ethanolamine respectively. On the other hand, the oil components like asphatenes, resins, aromatics and resins were simulated by different arrangements of aromatic and aliphatic beads in the DPD simulations. The simulations were carried out with Accelrys DPD package with a reduced parameter kBT = 1. The pair interaction parameters aij were calculated through the relationship between the Flory-Huggins solubility parameter:

$$a_{ij} = 25+3.50\chi \qquad (1)$$

Figure 1 displays the configurations of all the components used in the DPD calculations. In particular in Figure 1(a) is observed the presence of the copolymer in the interface oil/water.

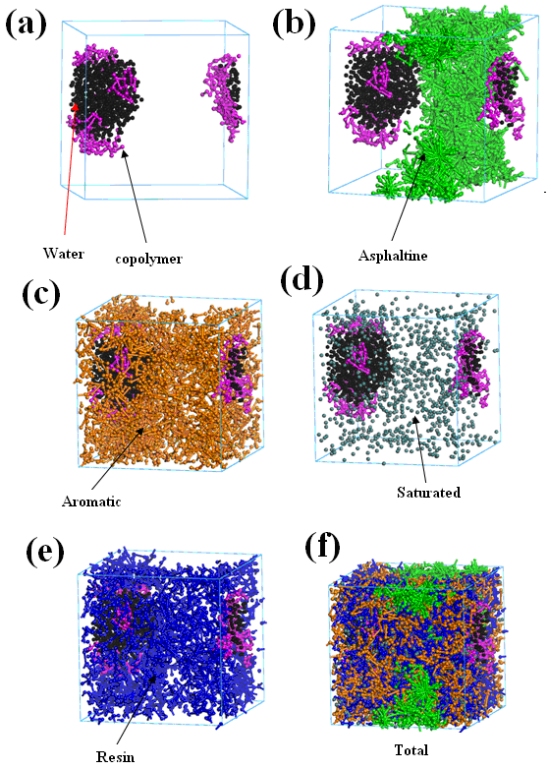

Fig. 1. Snapshots of (a) relative position of water and functionalized copolymer.(b-e) Asphaltene, aromatic, saturated and resin morphology in the stabilized fluid. (f) snapshot of all the components in the simulation.

References

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