Effect of Asphaltene Structure on Association and Aggregation with oleic acid using Molecular Dynamics

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In the present investigation the effects produced by the presence of alien molecules on the self-assembly of representative asphaltene molecules has been investigated by means of molecular dynamics (MD) technique. Two representative asphaltene molecules have been modelled according to structures from Venezuelan crude oils. The alien molecules considered for the simulations were belonging to the two currently used classes of molecules of long-chained carboxylic acids and alkylamines. Specifically, we have chosen for our studies oleic acid and bis (2-ethyl hexyl) amine because we consider they may have enhanced performances due to their peculiar structures. The results will be used to understand the structural and dynamical factors influencing the asphaltene aggregation thus helping to choose of ad-hoc bitumen additives. future directions in the piloted design of ad-hoc bitumen additives.