

Study on the aggregate structure and stability of heavy crude oil using a DPD based meso-platform

Junbo Xu^a, Shengfei Zhang^{a,b}, Hao Wu^a, Hao Wen^{a,*}

^a State Key Laboratory of Multi-Phase Complex System, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, P.R. China (* corresponding author: hwen@home.ipe.ac.cn)

^b Graduate University of Chinese Academy of Sciences, Beijing 100049, P.R. China

The research interest on heavy crude oil is increasing as the reservoir of conventional crude oil decreased. The aggregate structure of heavy crude oil, influencing the rheology, dispersity, stability of water-in-oil emulsions, poisoning of catalysts, fouling of hot metal surfaces, extent of wettability alteration, attracts much industrial attention.

In this work, aggregate behaviour of asphaltenes in heavy crude oil was explored by a DPD (Dissipative Particle Dynamics) based mesoscale platform. GPU (Nvidia[®] GTX285 graphics card) was used to accelerate the simulation, which gains over 20x speedup against the serial version DPD provided by Materials Studio and over 10x speedup against the parallel version of DPD provided by CULGI running on 5 CPU cores; rigid body fragments, which represents the significant presence of fused aromatic rings structure in fractions such as asphaltenes and resins, was introduced into DPD.

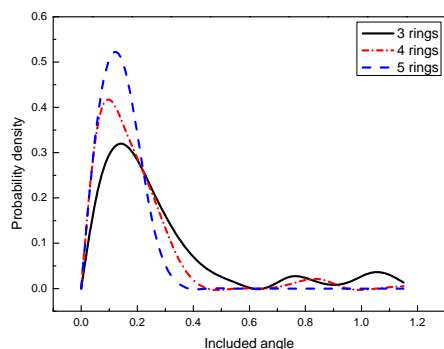


Fig. 1. The included angle distributions of 3-ring, 4-ring and 5-ring model molecules of asphaltenes

Three sets of asphaltene model molecules, containing 3, 4 and 5 coarse-grained fused aromatic rings individually, were considered with continental model in simulation. Face to face, offset and T-shaped aggregate structures were observed, similar to those researches done by MD [1]. The distributions of included angle (Fig. 1), the angle between rigid sheets of asphaltene model molecules in a designed distance, show that distribution peaks appeared at ~0.8 and ~1.1 radian in the case of 3-ring model molecules, which indicates some irregular structures or T-shaped geometry occurred in asphaltene aggregates. For 5-ring model molecules, the included angles appear mainly in range of 0 ~ 0.2 radians, reflecting the well-ordered aggregates. The aggregate

structures of 4-ring model molecules is better ordered than 3-ring model molecules and worse than 5-ring. The interlayer distance in well-ordered structure obtained from simulation is near 0.36 nm no matter which kind of model molecules, which agree with experimental data [2] well.

The cluster size of asphaltene molecules was used to represent the stability of crude oil. Fig.2 shows the stability predictions of 230 simulation systems: in zone A, the crude oil will keep stable in the whole range of saturate/aromatic ratio, clarifying the stability of crude oil is independent on the concentration of saturate or aromatic because of the dispersive action of enough resin; in zone B, there is not enough resin to disperse asphaltene clusters and thus the ratio of saturate/aromatic must be limited to low values to maintain the oil stable; zone C is considered as a part of stable phase when the ratio of saturate/aromatic is set to an exceedingly low value. The relationship between concentration and stability of crude oil is consistent with Shell's work [3].

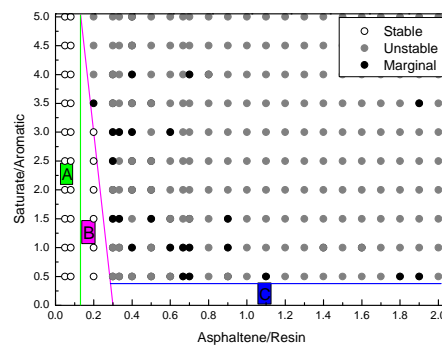


Fig. 2. A cross-plot of heavy crude oil from simulations

Acknowledgments:

We acknowledge financial support through the National Natural Science Foundation of China (project 20776141 and 20821092).

References

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