Supporting Information

Characterizing Asphaltene Deposition in the Presence of Chemical Dispersants in Porous Media Micromodels

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S1. Images of Asphaltene Aggregates from Optical Microscopy and SEM

No particle is observed from images measured by optical microscopy under the same condition as used in DLS measurements as shown in Figure S1. The aggregates are also measured by SEM and globular shape is obtained as shown in Figure S2.



Figure S1. Microscopic images for asphaltene aggregates. (a) No dispersant. (b) *p*-dodecylphenol. Scale bar is 50 μm.



Figure S2. SEM images for asphaltene aggregates. (a) No dispersant. (b) *p*-hexylpheno. (c) *p*-octylphenol. (d) *p*-dodecylphenol. (e) *iso*-dodecylphenol. Scale bar is 5 μ m.

S2. Numerical Simulation on Flow through Porous Media

To obtain the insight into the velocity field and the shear rate inside the porous media microfluidic channel during asphaltene deposition experiments, a numerical model based on the Lattice-Boltzmann method (LBM) is performed. The present model describes the steady flow of fluids in a representative elementary volume (REV) of the homogeneous porous media pattern. The LBM simulation is carried out in two dimensions. Because the depth of the microchannel is much smaller than the width/length of it, the 2-D calculation should be close to the real scenario. An open source code, Palabos (http://www.palabos.org/) was adapted to perform the LBM simulation. A real picture of the REV from the deposition experiment was first digitalized to a binary mask to be used as the simulation domain, in which both the stationary circular grain and the asphaltene deposits was treated as solid wall with no-slipping boundary conditions. The constant average injection velocity was set at the

inlet of the REV domain, periodic boundary conditions was set at both upper and lower sides of the REV domain, and a pressure outlet boundary condition was set at the outlet of the REV domain. The time-transient LBM simulation was performed until the relative error between time steps was less than 10⁻⁴, at which we concluded the steady state had been reached. Finally, the simulation data was analyzed in the ParaView software from which the velocity field and the shear rate distribution was calculated and plotted.

S3. Parameters for Steric Repulsion Approximation

The distance between attachment points (*s*) was estimated with the method by Rahme *et al*¹, which is the square root of the surface area for the asphaltene aggregate per dispersant molecule, and the distances were 6.55 nm for *p*-hexylphenol, 7.05 nm for *p*-octylphenol, and 7.95 nm for *p*-dodecylphenol with the assumption that all the dispersants in the oil adsorbed on asphaltenes. The thickness of the adsorbed layer (*L*) was taken as size of the dispersant, and they were estimated to be 1.18 nm for *p*-hexylphenol, 1.39 nm for *p*-octylphenol, and 1.89 nm for *p*-dodecylphenol by Gaussian G09.D1. The volume and the surface area of an asphaltene molecule were estimated by Eq. S1 and Eq. S2. The distance between attachment points was estimated by Eq. S3 with the assumption of a spherical shape for the asphaltene aggregate.

$$V_A = \frac{M_w}{\rho_A \cdot N_A} \tag{S1}$$

$$A_{s} = \left(36\pi V_{A}{}^{2}\right)^{\frac{1}{3}}$$
(S2)

$$s = \left(A_s \cdot \frac{\text{mole of asphaltenes}}{\text{mole of dispersants}}\right)^{\frac{1}{2}}$$
(S3)

where V_A is the volume of an asphaltene molecule, M_w is the molecular weight of the asphaltene aggregate (4000 g/mol), ρ_A is the density of the asphaltene (1.2 g/cm³), N_A is the Avogadro number, and A_s is the surface area of the asphaltene aggregate.

S4. Videos of Deposition

Video S1 is for *p*-octylphenol and video S2 is for *p*-dodecylphenol.

References

Rahme, K.; Chen, L.; Hobbs, R. G.; Morris, M. A.; O'Driscoll, C.; Holmes, J. D. *RSC Adv.* 2013, *3* (17), 6085.