SUPPLEMENTARY MATERIAL

Mesoscale computer modeling of asphaltene aggregation in liquid paraffin

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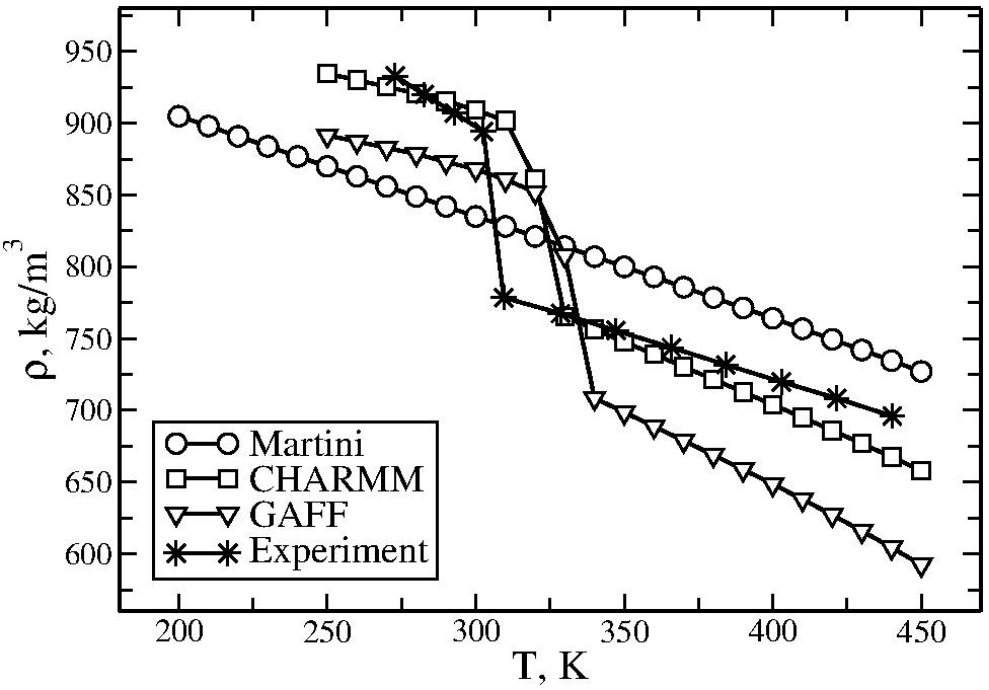

FIG. S1. Mass density of n-eicosane as a function of temperature. Shown are results for the Martini simulations, for the CHARMM36 and GAFF all-atom simulations,[1] as well as the experimental data.[2]

TABLE SI. Refined Lennard-Jones parameters used for coarse-grained simulations of paraffin-asphaltene systems. The original Martini parameters[3] are presented in brackets (where applicable).

	σ [nm]	ε [kJ/mol]
C1-C1	0.47	3.5
SC5-SC5	0.35 (0.43)	1.6 (2.625)
SC5-C1	0.43 (0.47)	2.25 (3.1)

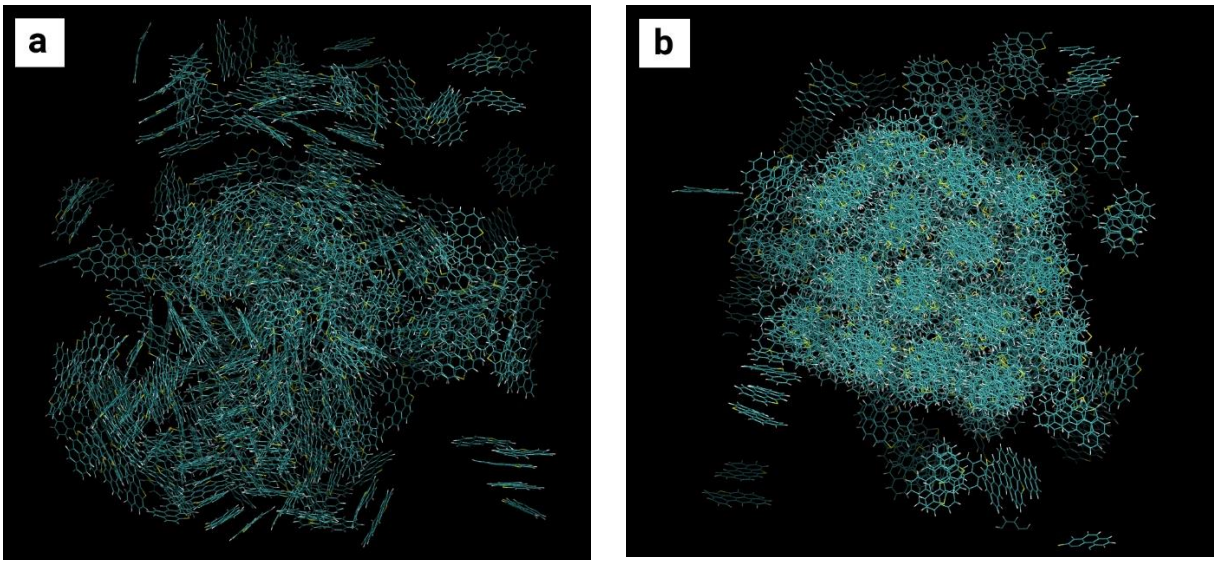

FIG. S2. (a) A snapshot of the PAR-ASPM-44 system in atomistic simulations (the GAFF force field).[4] (b) A snapshot of the same system after GAFF charges were replaced with CHARMM36 charges. Modified asphaltenes are shown in cyan; paraffin chains are not shown for clarity.

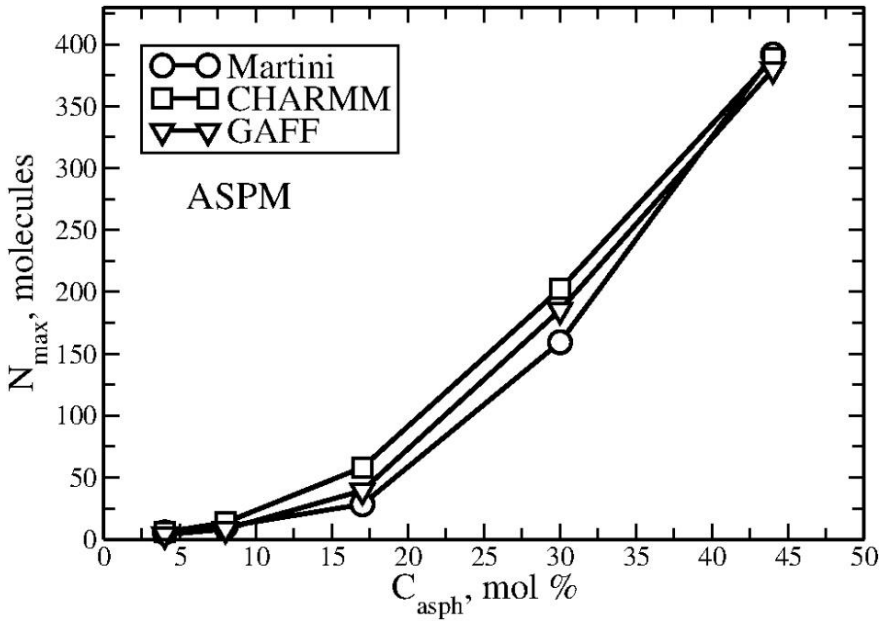

FIG. S3. The average number N_{max} of asphaltene molecules in the largest aggregate as a function of the concentration of modified asphaltenes (ASPM) in the system. Shown are results for the coarse-grained Martini force field as well as the atomistic CHARMM36 and GAFF force fields.

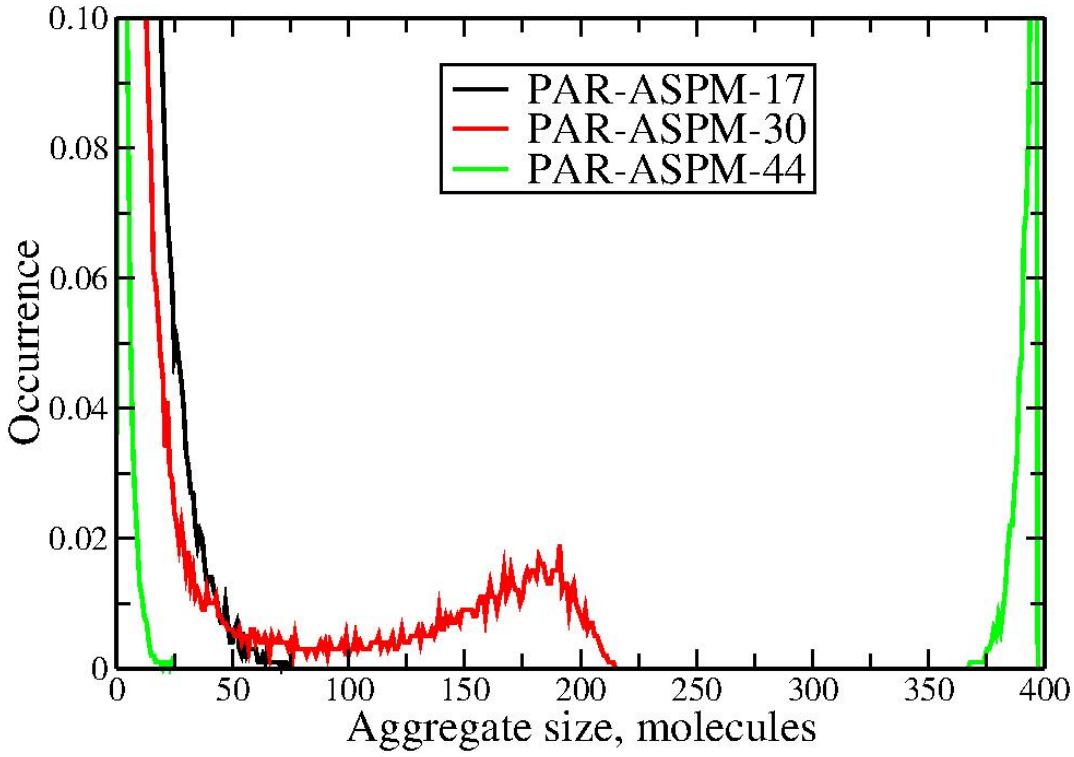

FIG. S4. The distribution of modified asphaltenes over aggregate sizes. Shown are results for the PAR-ASPM-17, PAR-ASPM-30, and PAR-ASPM-44 systems.

References

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[2] W.F. Seyer, R.F. Patterson, and J.L. Keays, The density and transition points of the n-paraffin hydrocarbons, J. Am. Chem. Soc. 66, 179 (1944). https://doi.org/10.1021/ja01230a004

[3] S.-J. Marrink, H.J. Risselada, S. Yefimov, D.P. Tieleman, and A.H. de Vries, The Martini force field: coarse grained model for biomolecular simulations. J. Phys. Chem. B 111, 7812 (2007). https://doi.org/10.1021/jp071097f

[4] A.D. Glova, V.M. Nazarychev, S.V. Larin, A.V. Lyulin, S.V. Lyulin, and A.A. Gurtovenko, Asphaltenes as novel thermal conductivity enhancers for liquid paraffin: insight from *in silico* modeling, J. Mol. Liq. 346, 117112 (2022). https://doi.org/10.1016/j.molliq.2021.117112