Supplementary Information

Influence of Solvent Effect, Temperature, and Pressure on the Aggregation Behavior of Island Model Asphaltene: A Molecular Dynamics Study

Cun Hu [a,b,c*], Dandan Hong [a,b,c], E Fu [a,b,c], Yalou Sun [a,b,c], Jipeng Wang [a,b,c],Li Chen [a],Xiaoyu Hu [a,b,c], Jun Wang [a,b,c], Zhaohui Hu [a,b,c], Wenjing Shi [a,b,c], Zhi Cao [a,b,c], Yiqiang Zhong [a,b,c], Changchun Wang [a,b,c], Lulu Hu [a,b,c*]

[a] The 404 Company Limited, China National Nuclear Corporation, Jiayuguan 735100, China.

[b] Key Laboratory of Nuclear Fuel Cycle Technology, The 404 Company Limited, China National Nuclear Corporation, Lanzhou 735100, China.

[c] Chengdu Nuclear Engineering Design & Research Institute Co., Ltd., 404., CNNC, Chengdu, 610000, China.

* Corresponding author: E-mail: hucun402@163.com (C. Hu), L_L_Hu@163.com (LL Hu)

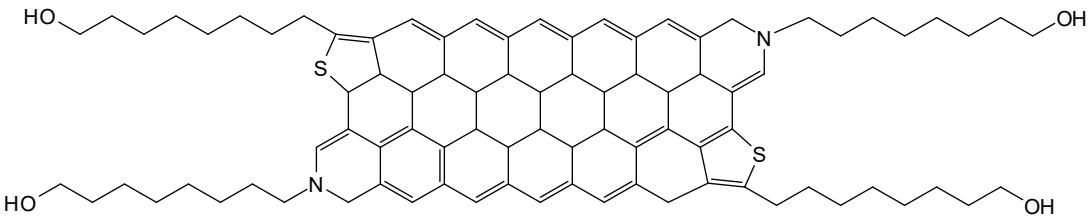

Figure S1：2D structural diagram of the asphaltene molecular model.

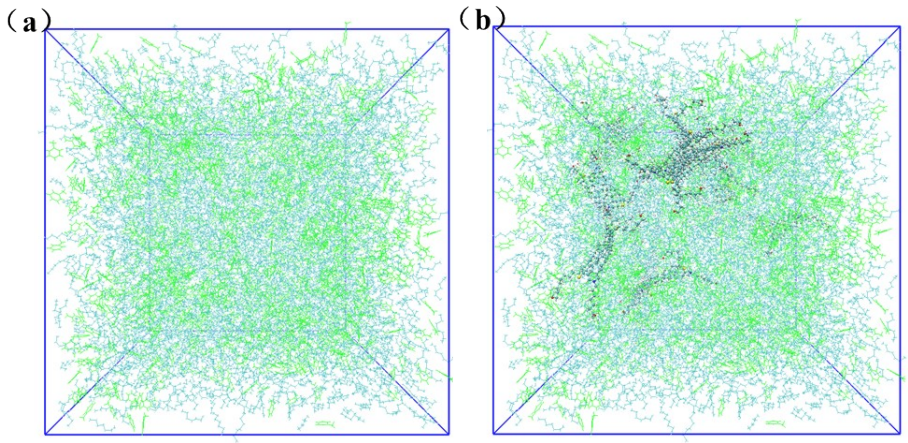

Figure S2：Simulation system: (a)70% n-heptane + 30% toluene system; (b) 70% n-heptane + 30% toluene + asphaltene system (n-Heptane molecules are shown in cyan, toluene molecules in green, and ASP1 molecules in a ball-and-stick model).

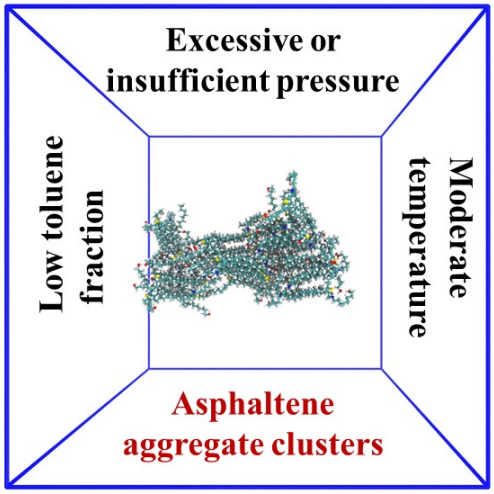

Figure S3：Stacked asphaltene structures and their behavior in solvents.

Table S1. The composition and dimensions of different solvent simulation systems (P =1 bar (0.1 MPa), T = 60℃ (333 K)).

Toluene mass fraction	Number of n-heptane molecules	Number of toluene molecules	Number of asphaltene molecules	Initial dimension of the system model	Final dimension of the system model
10%	4590	555	22	12.0 nm ×12.0 nm ×12.0 nm	10.96 nm ×10.97nm ×10.96 nm
20%	4080	1110	22	12.0 nm ×12.0 nm ×12.0 nm	10.87 nm ×10.87 nm ×10.87 nm
30%	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.78 nm ×10.77 nm ×10.77 nm
40%	3054	2224	22	12.0 nm ×12.0 nm ×12.0 nm	10.68 nm ×10.67 nm ×10.67 nm
50%	2550	2772	22	12.0 nm ×12.0 nm ×12.0 nm	10.56 nm ×10.57 nm ×10.56 nm

Table S2. The composition and dimensions of simulation systems at different temperatures (P =1 bar (0.1 MPa), 30% toluene).

Temperature	Number of n-heptane molecules	Number of toluene molecules	Number of asphaltene molecules	Initial dimension of the system model	Final dimension of the system model
30°C (303K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.61 nm ×10.61 nm ×10.61 nm
40°C (313K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.66 nm ×10.66 nm ×10.66 nm
50°C (323K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.71 nm ×10.71 nm ×10.71 nm
60°C (333K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.78 nm ×10.77 nm ×10.77 nm
70°C (343K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.82 nm ×10.81 nm ×10.82 nm
80°C (353K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.89 nm ×10.89 nm ×10.89 nm
90°C (363K)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.92 nm ×10.91 nm ×10.91 nm

Table S3. The composition and dimensions of simulation systems at different pressures (T = 60 ℃ (333 K), 30% toluene).

Pressure	Number of n-heptane molecules	Number of toluene molecules	Number of asphaltene molecules	Initial dimension of the system model	Final dimension of the system model
0.1MPa (1bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.78 nm ×10.77 nm ×10.77 nm
0.5MPa (5bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.76 nm ×10.76 nm ×10.76 nm
1MPa (10bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.75 nm ×10.75 nm ×10.75 nm
2MPa (20bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.74 nm ×10.74 nm ×10.74 nm
5MPa (50bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.73 nm ×10.73 nm ×10.73 nm
8MPa (80bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.71 nm ×10.71 nm ×10.71 nm
10MPa (100bar)	3580	1630	22	12.0 nm ×12.0 nm ×12.0 nm	10.72 nm ×10.72 nm ×10.72 nm