Supporting Information

Investigating the Applicability of Molecular Dynamics Simulation for Estimating the Wettability of Sandstone Hydrocarbon Formations

Vahid Khosravi*, Syed Mohammad Mahmood**, Davood Zivar, Hamid Sharifigaliuk

Petroleum Engineering Department, Universiti Teknologi PETRONAS, Perak, Malaysia

*Corresponding author email: vahid.khosravi87@gmail.com, vahid_17006746@utp.edu.my

**Corresponding author email: Mohammad.mahmood@utp.edu.my

Table S1. Trajectory documents of the different scenarios

Liquid	Number of fluid atoms	Number of total atoms of the system (fluids and polyethylene surface)	Size of Surface (polyethylene) (A*B*C each in Å) as amorphous cell	Amorphous Cell Volume (Å3)
n-pentane	17	637	19.7353*19.7353*19.7353	7686.52
n-hexane	20	640	19.4709*19.4709*19.4709	7381.76
n-heptane	23	643	19.2225*19.2225*19.2225	7102.84
n-octane	26	646	19.0782*19.0782*19.0782	6944.01
n-decane	32	652	18.8997*18.8997*18.8997	6750.99
cyclohexane	18	638	18.3733*18.3733*18.3733	6202.45
n-tetradecane	44	664	18.7317*18.7317*18.7317	6572.50
toluene	15	635	17.7456*17.7456*17.7456	5588.18
benzyl alcohol	16	636	16.7318*16.7318*16.7318	4684.16
ethylene glycol	10	630	16.2863*16.2863*16.2863	4319.84

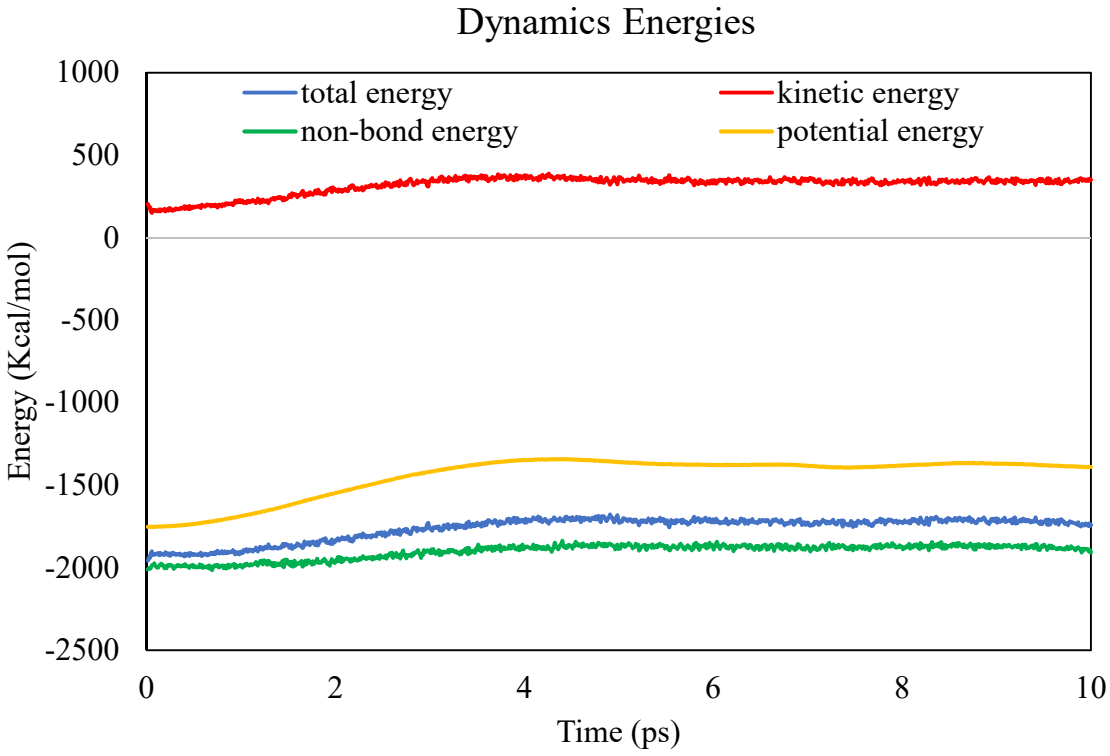

Figure S1. The dynamic energy of the system

Table S2. The molarity amounts of each concentration

NaCl brine concentration (ppm)	Molarity (mol/liter)
1,000	0.017
3,000	0.051
5,000	0.085
10,000	0.171
15,000	0.256