Supporting Information

Molecular Insight into Oil Displacement by CO_2 Flooding in the Water Cut Dead–end Nanopore

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Table S1. Lennard-Jones parameters employed in the simulations [1].

Atom type	ε (kJ/mol)	σ (nm)	q (e)
OB(O at SiO_2 bulk)	6.50629×10^{-1}	0.3166	-1.050
OS(O at SiO_2 surface)	6.50629×10^{-1}	0.3166	-0.950
Si	7.70581×10^{-6}	0.3302	2.100
H(at SiO_2 surface)	0.000	0.000	0.425
H(H_2O)	0.000	0.000	0.417
O(H_2O)	0.6364	0.315	-0.834
C(CO_2)	0.234	0.280	0.6516
O(CO_2)	0.6682	0.3028	-0.3258
CH_2	0.3808	0.393	0.000
CH_3	0.8647	0.391	0.000

Fig. S1. Snapshots of the systems with different water film thicknesses under 1 MPa during displacing process.

Fig. S2. Number density distribution of CO_2 and C10 perpendicular to the displacement direction in the groove with different water film thicknesses under the pressure of 1 MPa.

Fig. S3. The evolution of water film rupture at 4 MPa.

Fig. S4. The evolution of water film rupture at 1 MPa.

Fig. S5. The evolution of w–r H–bond number (a) and w–w H–bond number (b) during the simulations under the pressure of 1 MPa.

Fig. S6. The change of oil molecule number during the displacing process for different cases.

Fig. S7. Oil recovery for the cases with different water contents under 1 MPa and the corresponding fitting curves.

References

1 P. Lu, T. Mo, Y. Wei, Z. Guo and G. Feng, *J. Supercrit. Fluid.*, 2022, 181, 105507.