Supporting Information

Pore-scale Investigation of Carbon Dioxide Enhanced Oil Recovery

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1 Important setting and parameters

The CFD module of COMSOL Multiphysics is applied in this study (commercial software, which can directly implement partial differential equations and initial-boundary conditions). The COMSOL Multiphysics using a Galerkin finite element method to solve the N-S equation and phase field equation. An initial time step of 1×10^{-9} s is selected and the time step is allowed to automatically adjust based on the backward differentiation formula (BDF). A convergence criterion of 0.001 is specified to control the iterative solution process. PARDISO is used as a system solver. The parameters used in this software including the densities and viscosities of oil and water, the interface tension between oil and water, the mobility tuning parameter χ and the interface thickness ε. The density, viscosity and surface tension are determined by the type of fluid. Therefore, the only two parameters that may influence the reality and accuracy of solutions are the mobility tuning parameter χ and the interface thickness ε, which are manually selected. For the mobility tuning parameter χ,

$$\gamma = \chi\varepsilon^2 \tag{1}$$

Where γ is the mobility, $m^3 \cdot s/kg$; ε is the interface thickness, m. γ determines the time scale of the Cahn-Hilliard diffusion and it must be chosen judiciously. It must be large enough to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. Therefore, the mobility tuning parameter χ=1, which means $\gamma=\varepsilon^2$, is a good chose (COMSOL user's guide, Phase Field). In our simulations, we set χ=1 as the user's guide.

For the interface thickness ε, we set the interface thickness parameter to $\varepsilon=h_{max}/6$, where h_{max} is the maximum mesh size. So the interface thickness is determined by the grid size. To investigate the influence of the interface thickness on solutions (avoiding spurious solutions), we must test solutions in different elements (the effect of flow domain discretization).

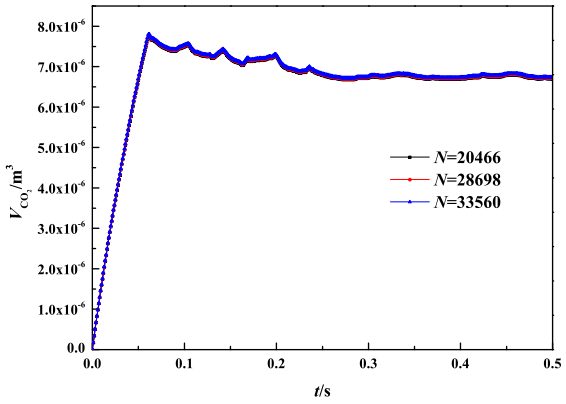

Figure S1 The CO2 volume with different elements

We can conclude that the porous media almost has the same CO_2 volume in different mesh-accuracy (The number of elements used in our study is 20466), which indicates that the parameters and solutions used in this study are reliable.

2 Simulation parameters

To help readers reproduce our results in section 3.2. The detailed simulation parameters are provided here.

2.1 Simulation parameters in section 3.2.1

The wetting angle of soil grain is $\theta=\pi/3$. The densities of oil and CO_2 are ρ_o=900 kg/m^3 and ρ_{CO2}=150 kg/m^3. The interface tension coefficient σ=0.025 N/m.

Table S1 The simulation parameters of section 3.2.1

U_{in}/m/s	μ_c /Pa·s	μ_o/ Pa·s	M	logCa
0.03	0.00002	0.02	0.001	-4.62
0.07	0.00002	0.02	0.001	-4.25
0.1	0.00002	0.02	0.001	-4.10
0.15	0.00002	0.02	0.001	-3.92
0.2	0.00002	0.02	0.001	-3.80
0.3	0.00002	0.02	0.001	-3.62

Where U_{in} is injection velocity, μ_c and μ_o are the viscosities of CO_2 and oil, respectively. M is the viscosity ratio and Ca is the capillary number.

2.2 Simulation parameters in section 3.2.2

The wetting angle of soil grain is $\theta=\pi/3$. The densities of oil and CO_2 are ρ_o=900 kg/m^3 and ρ_{CO2}=150 kg/m^3. The interface tension coefficient σ=0.025 N/m.

Table S2 The simulation parameters of section 3.2.2 (M=0.001)

U_{in}/m/s	μ_c/Pa·s	μ_o/ Pa·s	M	logCa
0.03	0.00002	0.02	0.001	-4.62
0.07	0.00002	0.02	0.001	-4.25
0.1	0.00002	0.02	0.001	-4.10
0.15	0.00002	0.02	0.001	-3.92
0.2	0.00002	0.02	0.001	-3.80
0.3	0.00002	0.02	0.001	-3.62

Table S3 The simulation parameters of section 3.2.2 (M=0.1)

U_{in}/m/s	μ_c/Pa·s	μ_o/ Pa·s	M	logCa
0.03	0.0001	0.001	0.1	-3.92
0.07	0.0001	0.001	0.1	-3.55
0.1	0.0001	0.001	0.1	-3.40
0.15	0.0001	0.001	0.1	-3.22
0.2	0.0001	0.001	0.1	-3.10
0.3	0.0001	0.001	0.1	-2.92

2.3 Simulation parameters in section 3.2.3

Table S4 The simulation parameters of section 3.2.3

U_{in}/m/s	θ	μ_c/Pa·s	μ_o/ Pa·s	M	logCa
0.07	45°	0.00005	0.005	0.01	-3.85
0.07	60°	0.00005	0.005	0.01	-3.85
0.07	75°	0.00005	0.005	0.01	-3.85
0.2	45°	0.00005	0.005	0.01	-3.40
0.2	60°	0.00005	0.005	0.01	-3.40
0.2	75°	0.00005	0.005	0.01	-3.40