

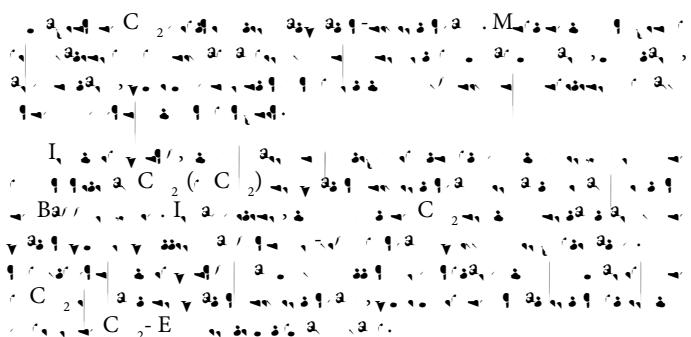
Impact of super-critical CO₂ on water/oil interfacial tension: A molecular dynamics case study

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Received: 1-Mar-2023, Manuscript No. ogr-23-88865; Editor assigned: 4-Mar-2023, PreQC No. ogr-23-88865 (PQ); Reviewed: 18-Mar-2023, QC No. ogr-23-88865; Revised: 25-Mar-2023, Manuscript No. ogr-23-88865 (R); Published: 31-



Methodology

Barro et al. (2016) studied the dissolution of BaCO_3 in supercritical CO_2 at 18 MPa and 293 K. They used a molecular dynamics simulation to model the dissolution process. The simulation results showed that the dissolution rate increased with increasing temperature and pressure. The dissolution mechanism was found to involve the formation of a supersaturated solution of Ba^{2+} and CO_3^{2-} ions in the supercritical CO_2 phase. The dissolution rate was found to be proportional to the square root of the dissolution time.

$$E_{vdW} = D_0 \left(2 \frac{\rho}{R} \frac{R_0}{R} \right)^2 + 43 \frac{\rho}{R} \frac{R_0}{R} \quad (4.1)$$

$$D = 0 \quad 0$$

F_n = 1.3, F_m = 1.3, P₀ = 252.53 MPa, T = 229.2 K, ρ_{oil} = 87.93 g/cm³, ρ_{water} = 1009 g/cm³, C₂ = 0.05 mol/L, A = 10 nm², L = 10 nm, $\gamma(t)$ = 17.252.53 MPa J (s)-229.2 K⁻¹ 87.93(1009 s)⁻¹.

$$\nu/t \equiv \left| \frac{d\gamma}{dt} \right| = \left| \frac{(P_{nn}/n, t) - 4P_{tt}/n, t)}{d_n} \right| \quad (4.3)$$

where $P_{nn}/n, t$ and $P_{tt}/n, t$ are the normal and tangential components of the pressure tensor at time t . The value of ν/t is 17.252.53 MPa J (s)-229.2 K⁻¹ 87.93(1009 s)⁻¹.

Table 1.2: Interfacial tension between liquid and vapor phases of pure hydrocarbons

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Component	5P1P simulation	Error	5P1P± Experiment ^{a,c}
Propane	9.85	0.302	10.1
Butane	13.3	0.23	12.46
Pentane	16.02	0.1	15.82
Hexane	18.41	0.12	18.43
Heptane	20.25	0.07	20.14
Octane	21.57	0.05	21.62

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Table 1.3: Interfacial tension between liquid and vapor phases of pure hydrocarbons

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Component	■ simulation ^b	Error	■ ± Experiment ^b
Propane	502.4	0.19	498
Butane	579.2	0.019	579
Pentane	627	0.045	626
Hexane	659	0.035	659.4
Heptane	684.1	0.048	683.7
Octane	705	0.059	703

b* engineering toolbox/ density/ alkanes

