

Supporting Information for “Interfacial Properties of H₂O+CO₂+Oil Three-Phase Systems: A Density Gradient Theory Study”

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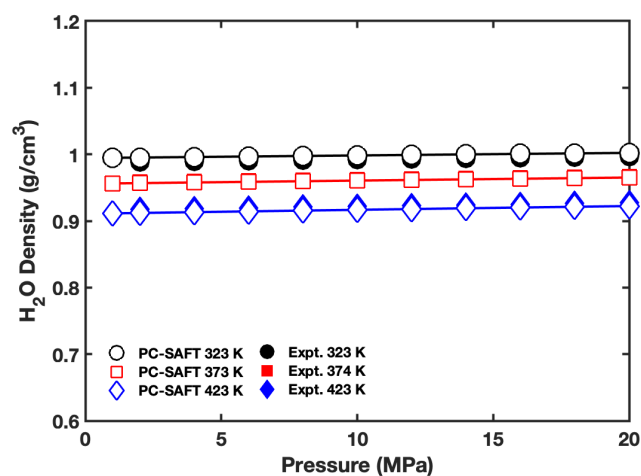


Figure S1: Densities of H₂O as a function of pressure at different temperatures. The experimental data from NIST (<http://webbook.nist.gov/chemistry/fluid>) are shown as solid symbols.

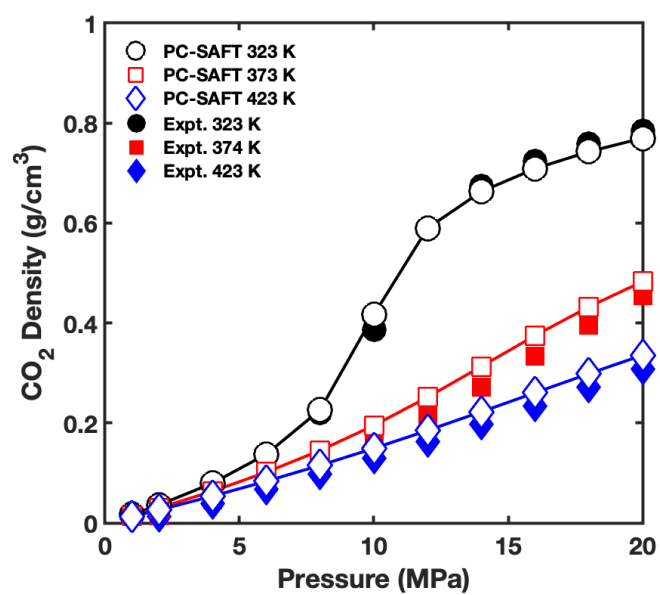


Figure S2: Densities of CO₂ as a function of pressure at different temperatures. The experimental data from NIST (<http://webbook.nist.gov/chemistry/fluid>) are shown as solid symbols.

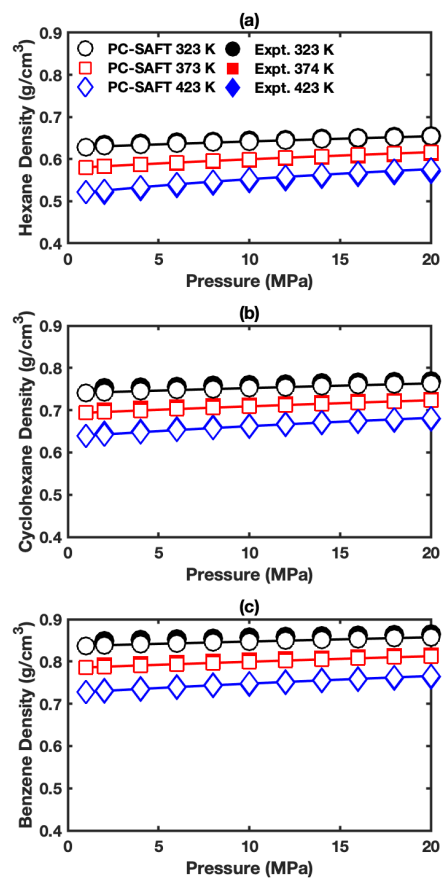


Figure S3: Densities of oil as a function of pressure at different temperatures. The experimental data from NIST (<http://webbook.nist.gov/chemistry/fluid>) are shown as solid symbols.

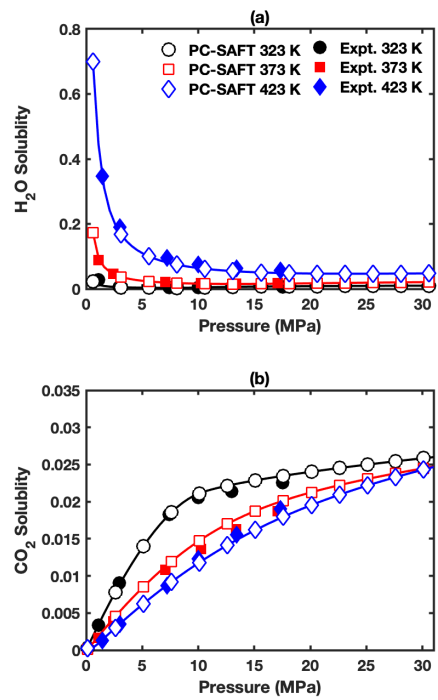


Figure S4: Solubilities in $\text{H}_2\text{O}+\text{CO}_2$ two-phase system. The experimental data is taken from (J. Supercrit. Fluids, 2013, 73: 87-96).

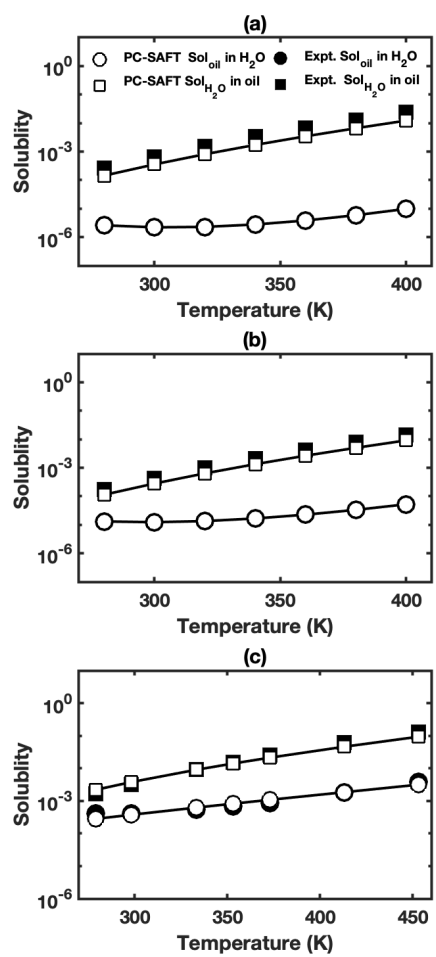


Figure S5: Solubilities in H_2O +oil two-phase system. The experimental data is taken from (J. Phys. Chem. Ref. Data, 2004, 33(2): 549-577) and (J. Chem. Eng. Data, 2003, 48(3): 750-752).

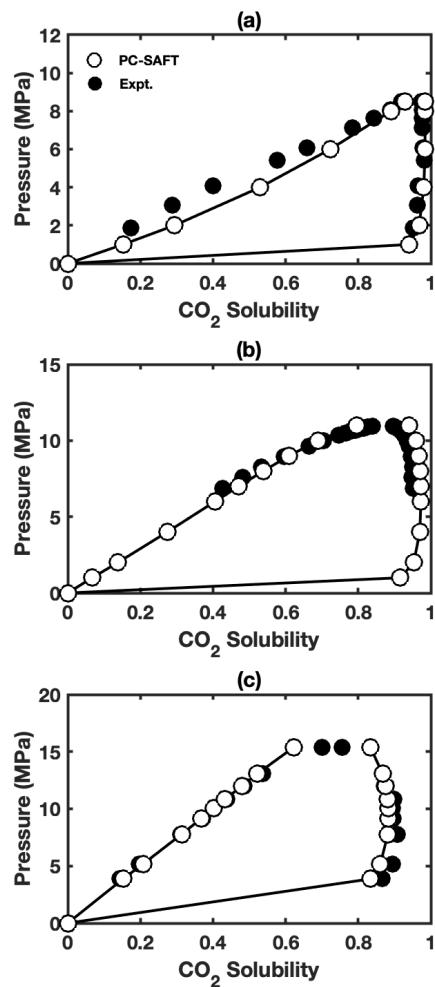


Figure S6: Solubilities in oil+CO₂ two-phase system. The experimental data is taken from (Fluid Phase Equilib., 1987, 33(1-2): 109-123), (J. Chem. Eng. Data, 1987, 32(3): 369-371), and (Fluid Phase Equilib., 1987, 36: 107-119).

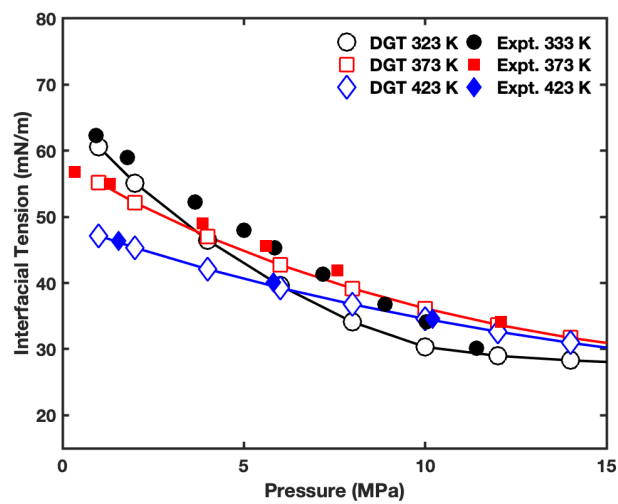


Figure S7: Pressure dependence of IFT in water-CO₂ two-phase system. The experimental data (J. Chem. Thermodyn., 2016, 93: 404) are shown as solid symbols.

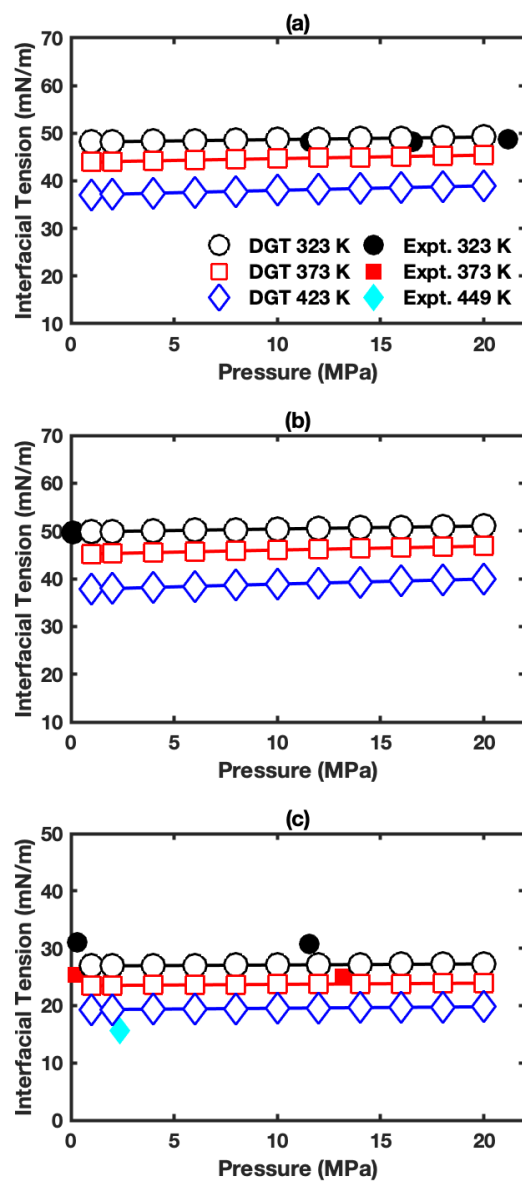


Figure S8: Pressure dependence of IFT in water+oil two-phase systems: (a) hexane; (b) cyclohexane; (c) benzene. The experimental data (J. Chem. Eng. Data, 1996, 41: 493; J. Phys. Chem., 1951, 55: 439; J. Colloid Interface Sci., 1967, 24: 323) are shown as solid symbols.

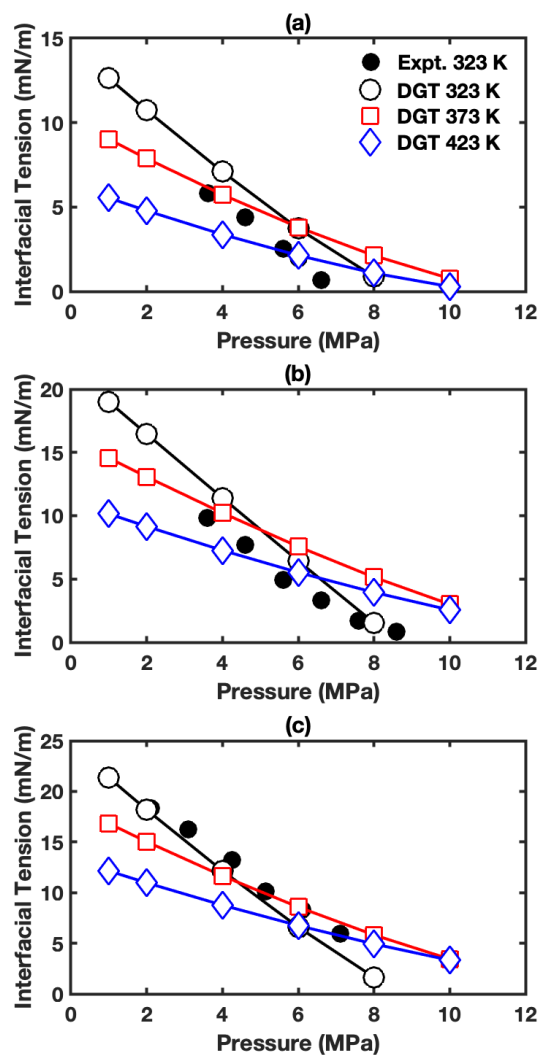


Figure S9: Pressure dependence of IFT in oil+methane two-phase systems: (a) hexane; (b) cyclohexane; (c) benzene. The experimental data (Chin. J. Chem. Eng., 2014, 22: 1302; J Supercrit Fluids, 2019, 154: 104625) are shown as solid symbols.

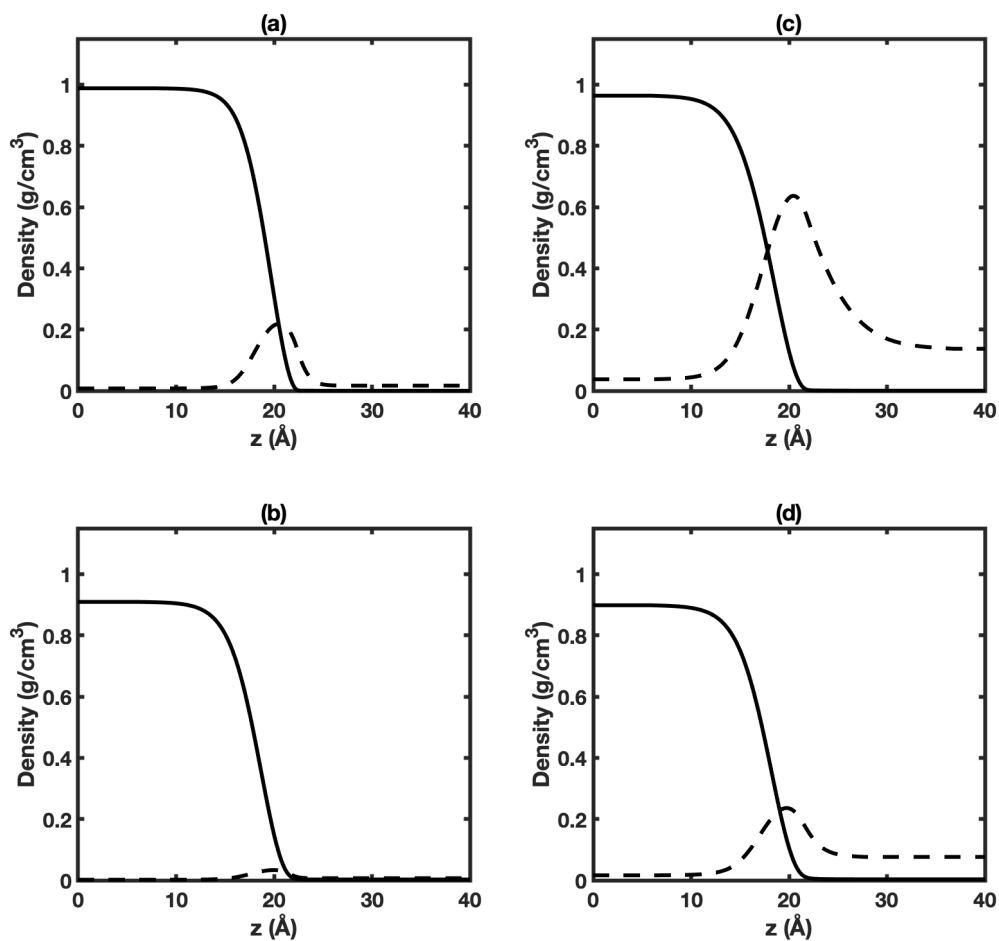


Figure S10: Equilibrium distributions of different species in water+CO₂ two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote water and CO₂, respectively.

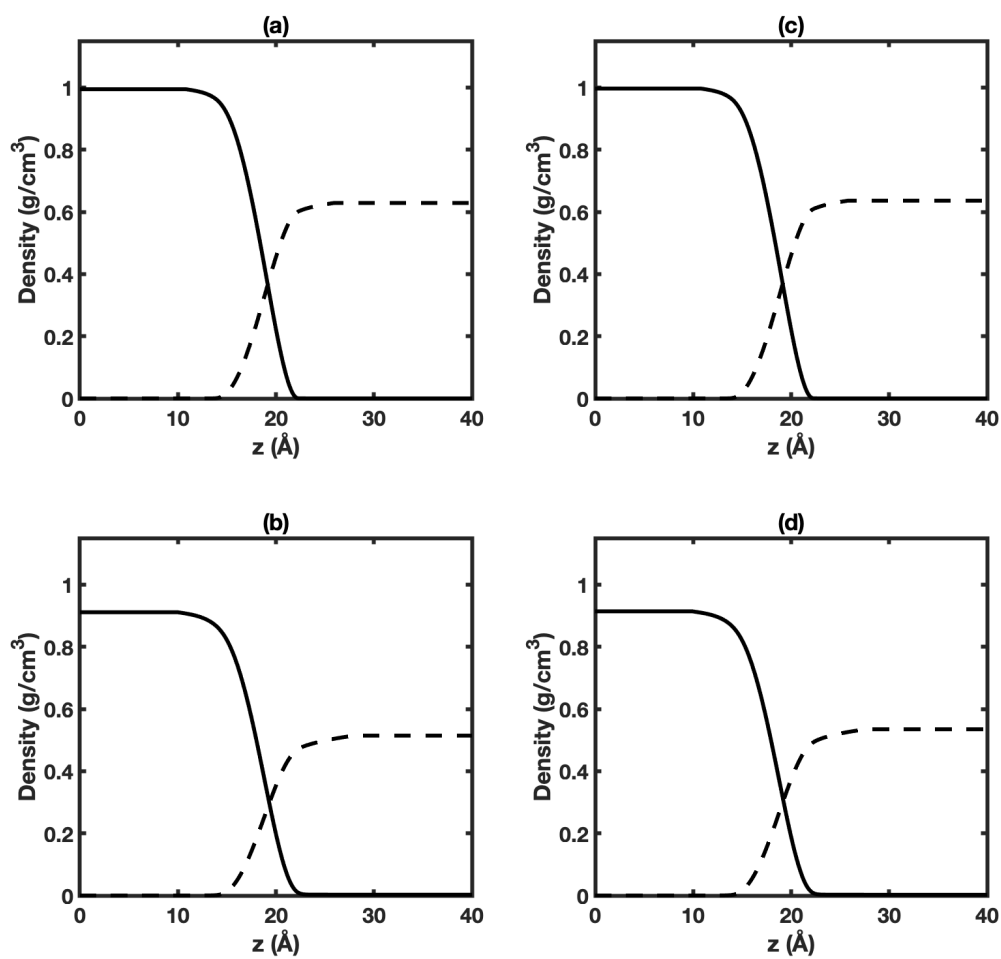


Figure S11: Equilibrium distributions of different species in hexane+water two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote water and hexane, respectively.

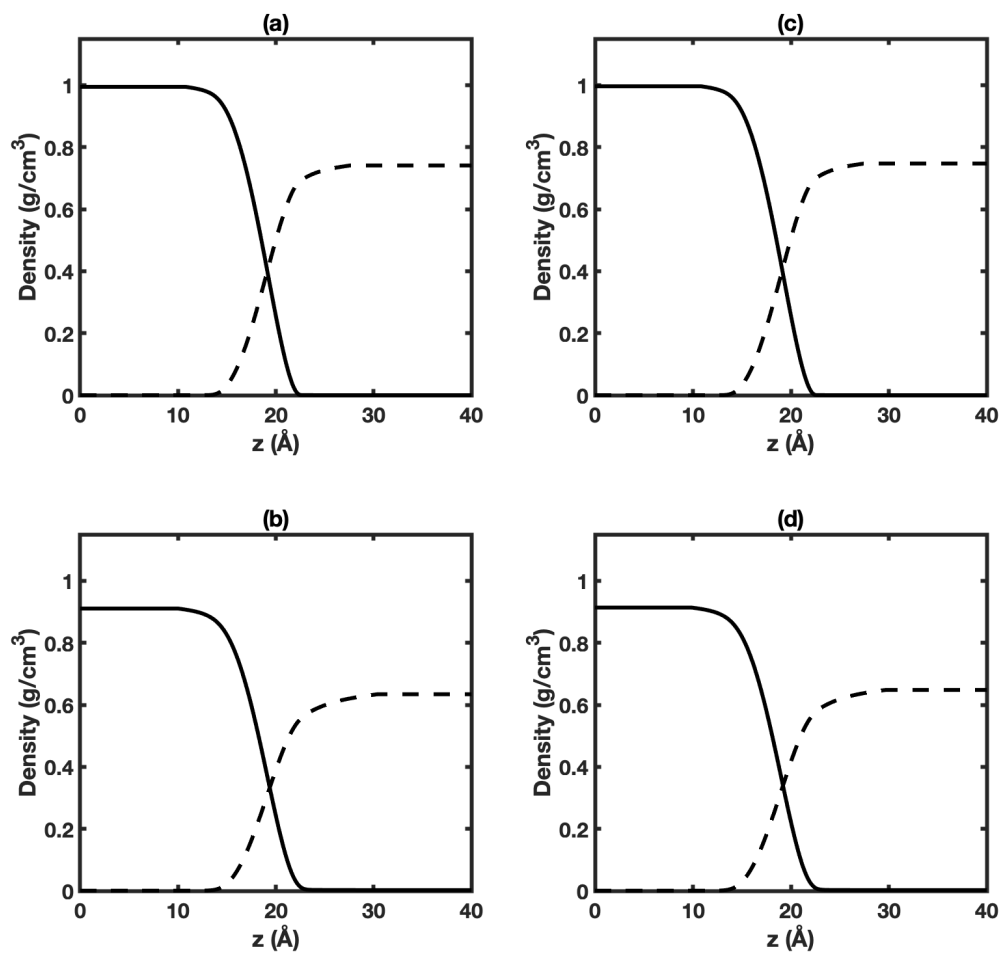


Figure S12: Equilibrium distributions of different species in cyclohexane+water two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote water and cyclohexane, respectively.

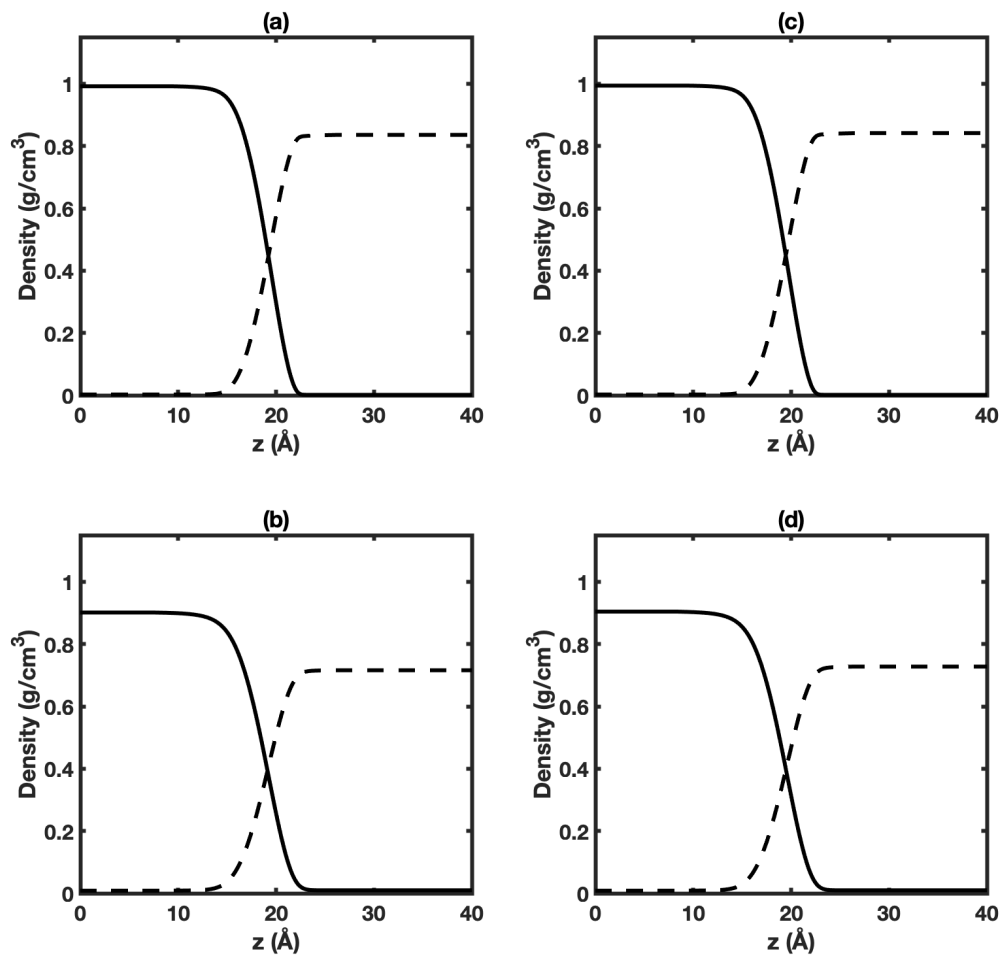


Figure S13: Equilibrium distributions of different species in benzene+water two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote water and benzene, respectively.

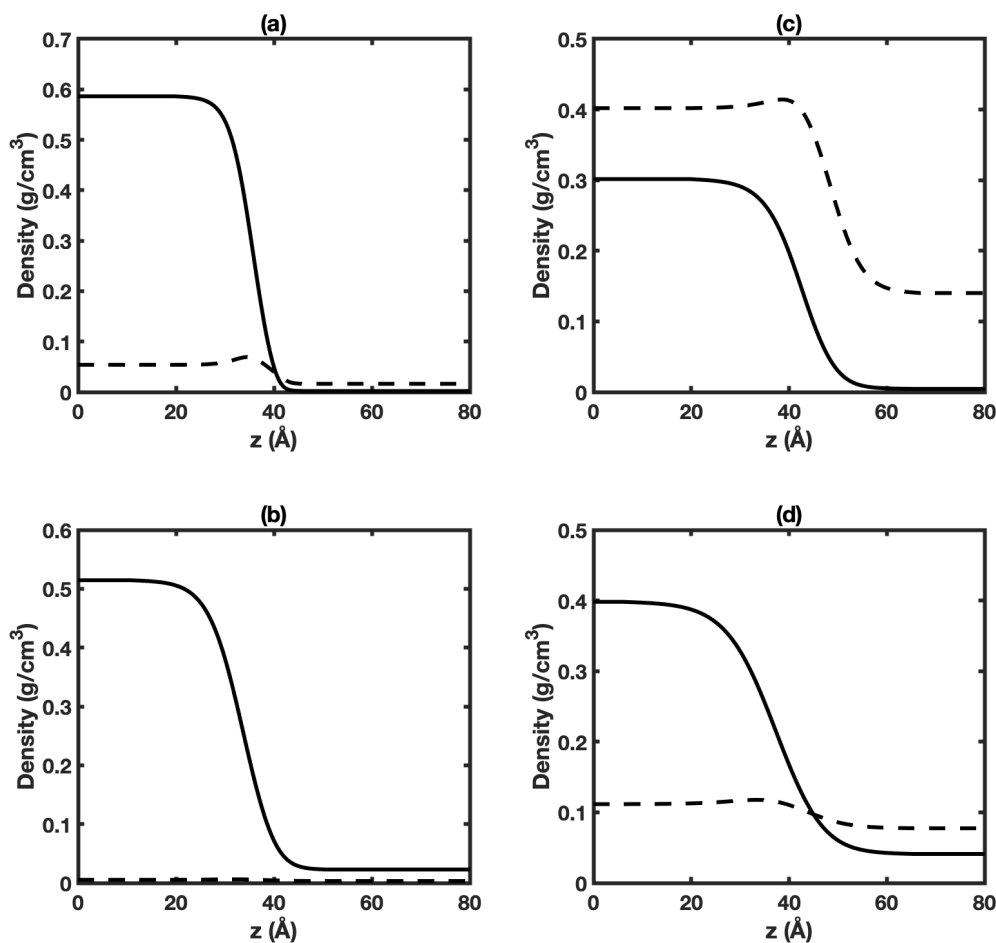


Figure S14: Equilibrium distributions of different species in hexane+CO₂ two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote hexane and CO₂, respectively.

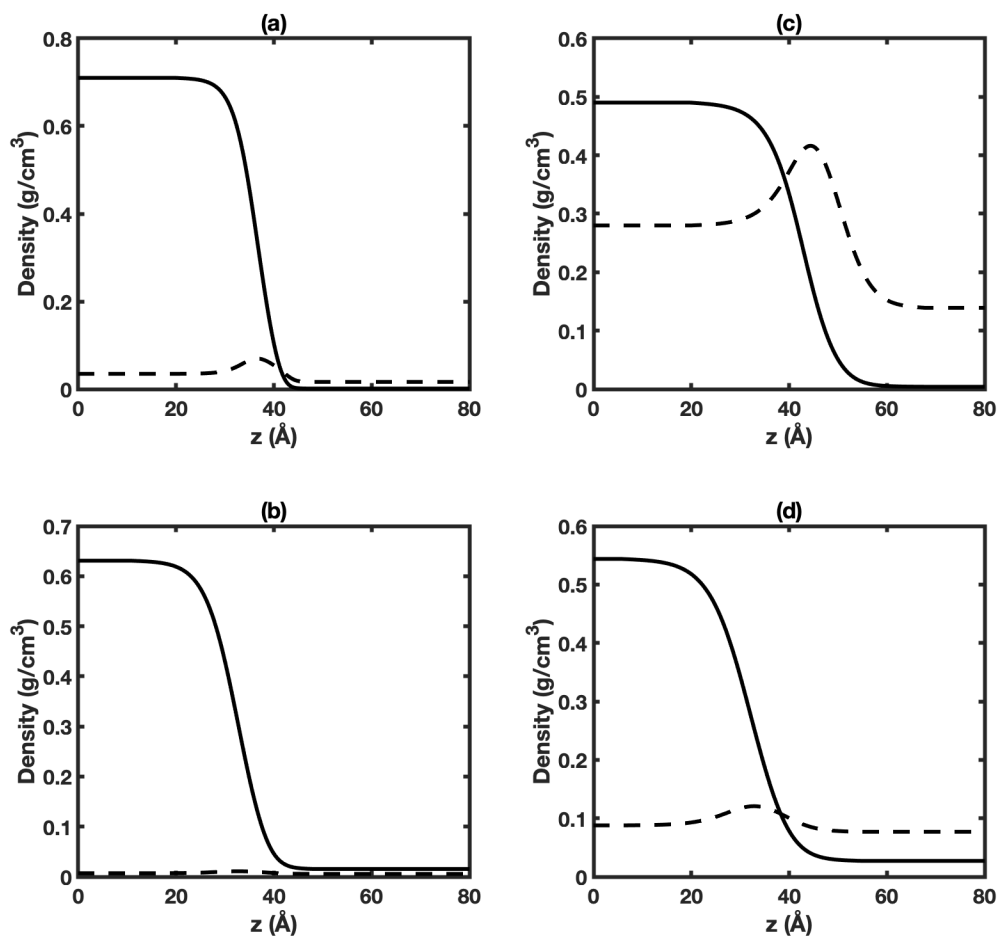


Figure S15: Equilibrium distributions of different species in cyclohexane+CO₂ two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote cyclohexane and CO₂, respectively.

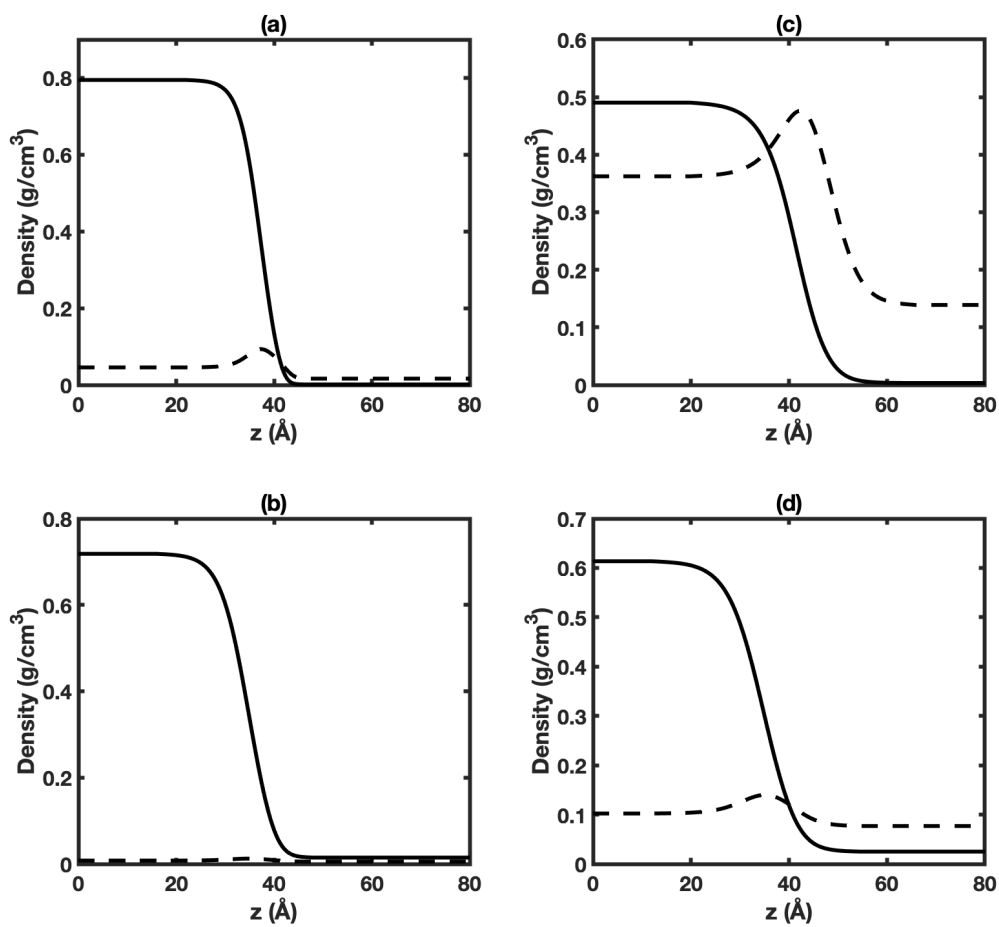


Figure S16: Equilibrium distributions of different species in benzene+CO₂ two-phase system at (a) 323 K and 1 MPa, (b) 423 K and 1 MPa, (c) 323 K and 6 MPa, and (d) 423 K and 6 MPa. The solid and dashed lines denote benzene and CO₂, respectively.

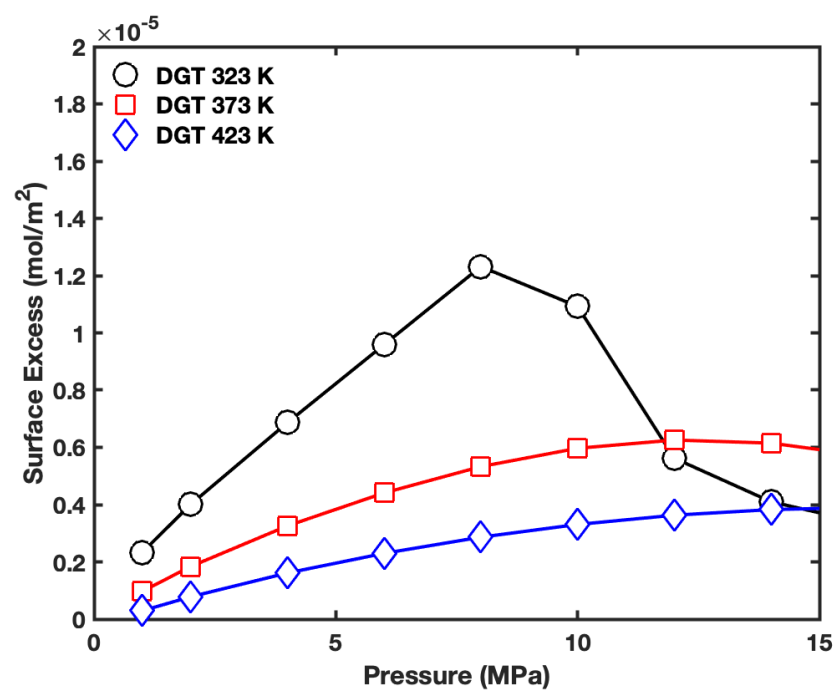


Figure S17: Pressure dependence of CO₂ surface excess in water+CO₂ two-phase system.

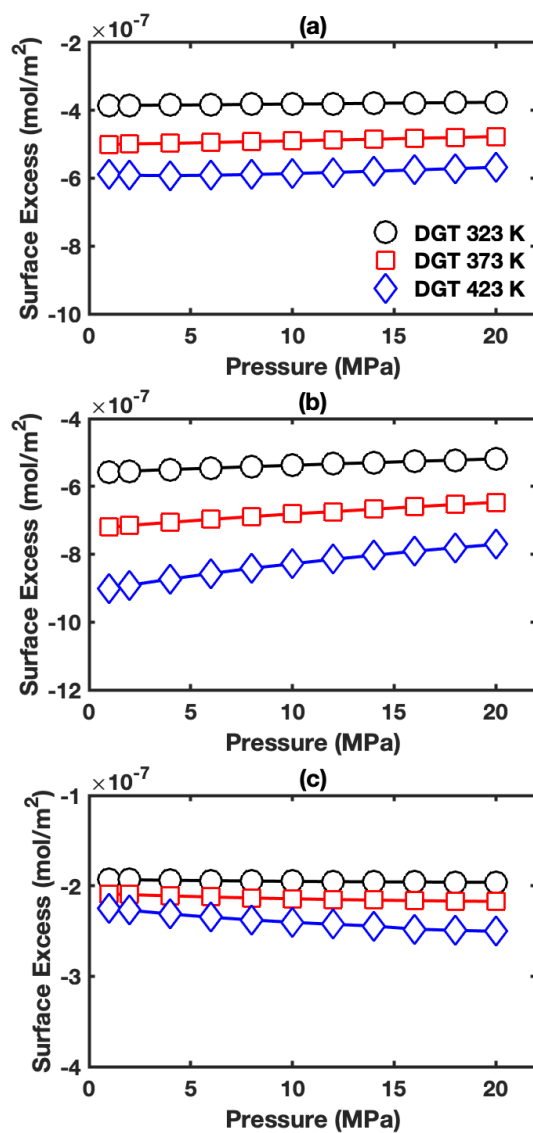


Figure S18: Pressure dependence of oil surface excess in water+oil two-phase systems: (a) hexane; (b) cyclohexane; (c) benzene.

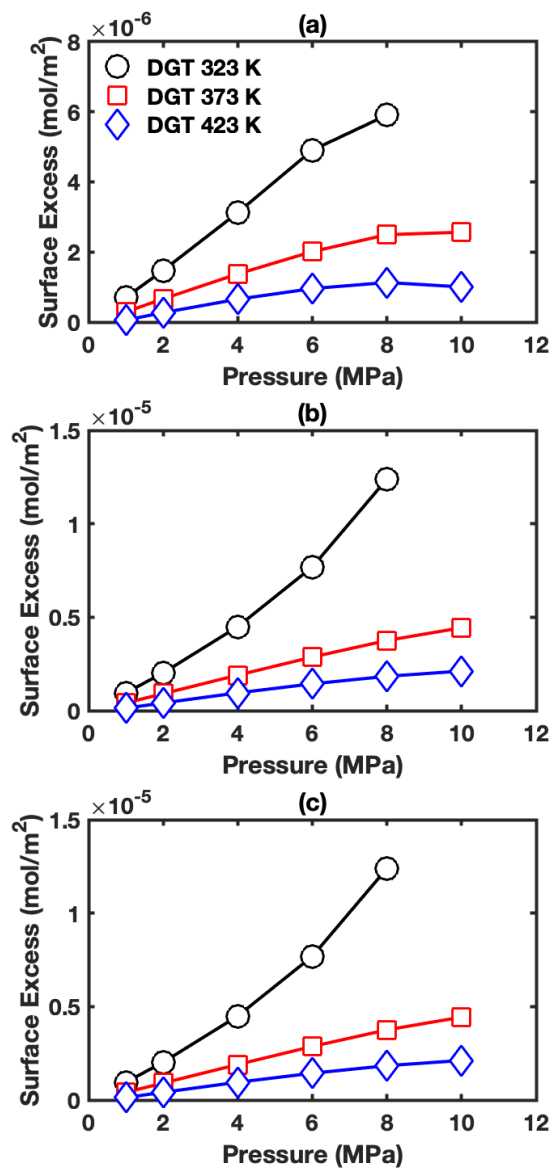


Figure S19: Pressure dependence of CO₂ surface excess in oil+CO₂ two-phase systems: (a) hexane; (b) cyclohexane; (c) benzene.

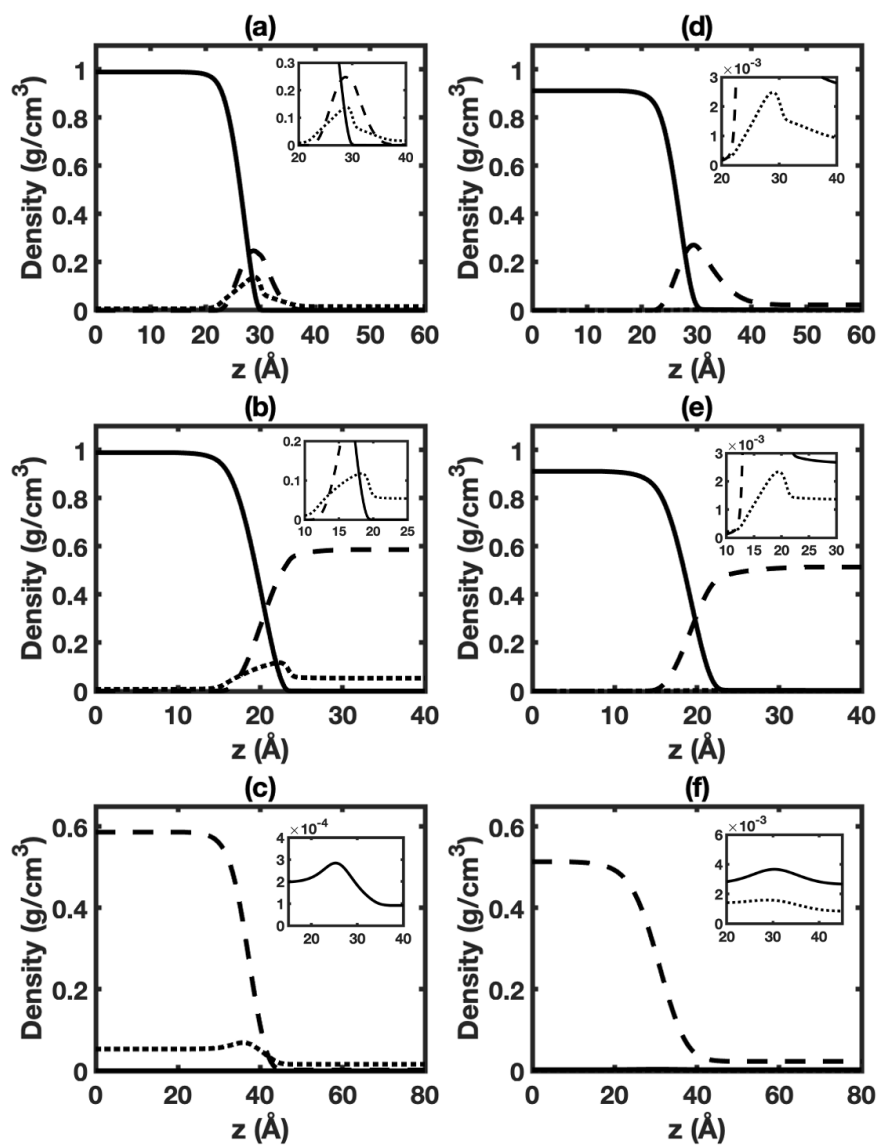


Figure S20: Same as Fig. 3, but at 1 MPa.

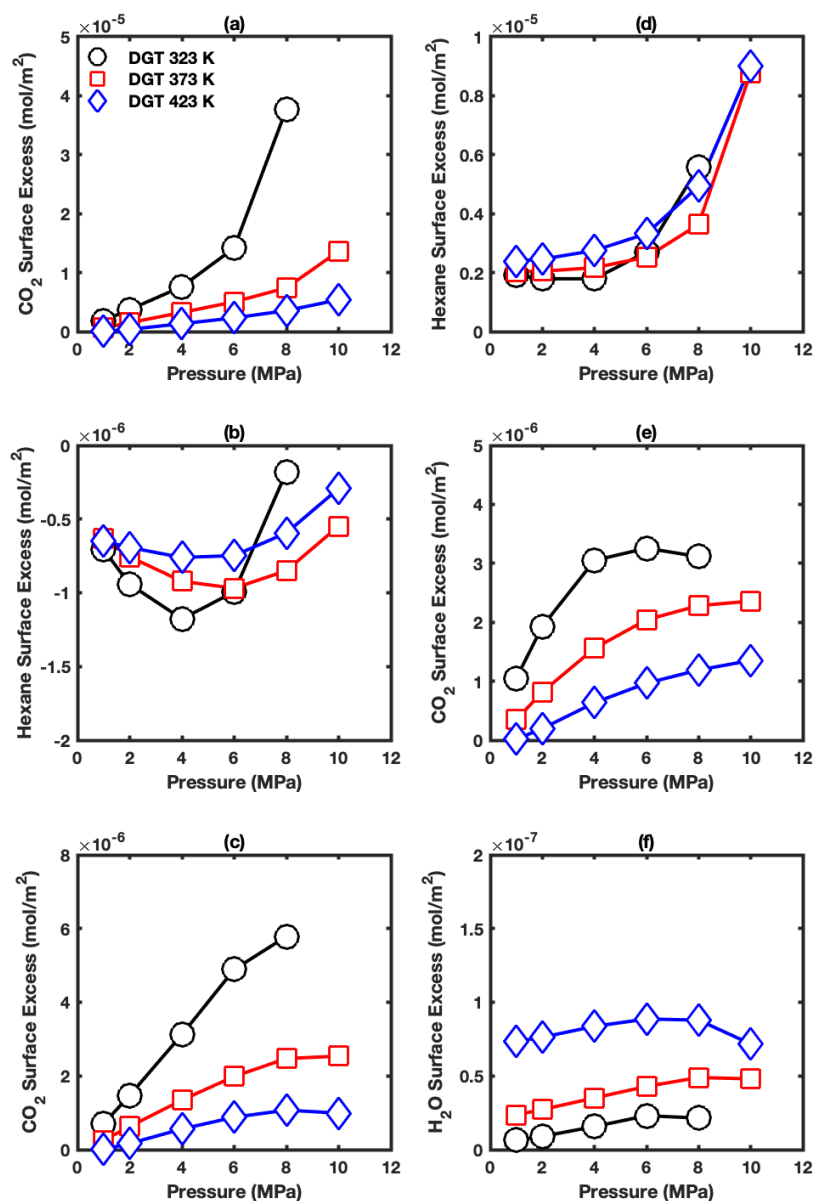


Figure S21: Pressure dependence of component surface excess in $\text{H}_2\text{O}+\text{CO}_2+\text{hexane}$ three-phase system: (a,d) interface of aqueous phase +vapor phase (top panels); (b,e) interface of aqueous phase+hexane-rich phase (middle panels); (c,f) interface of hexane-rich phase+vapor phase (bottom panels).

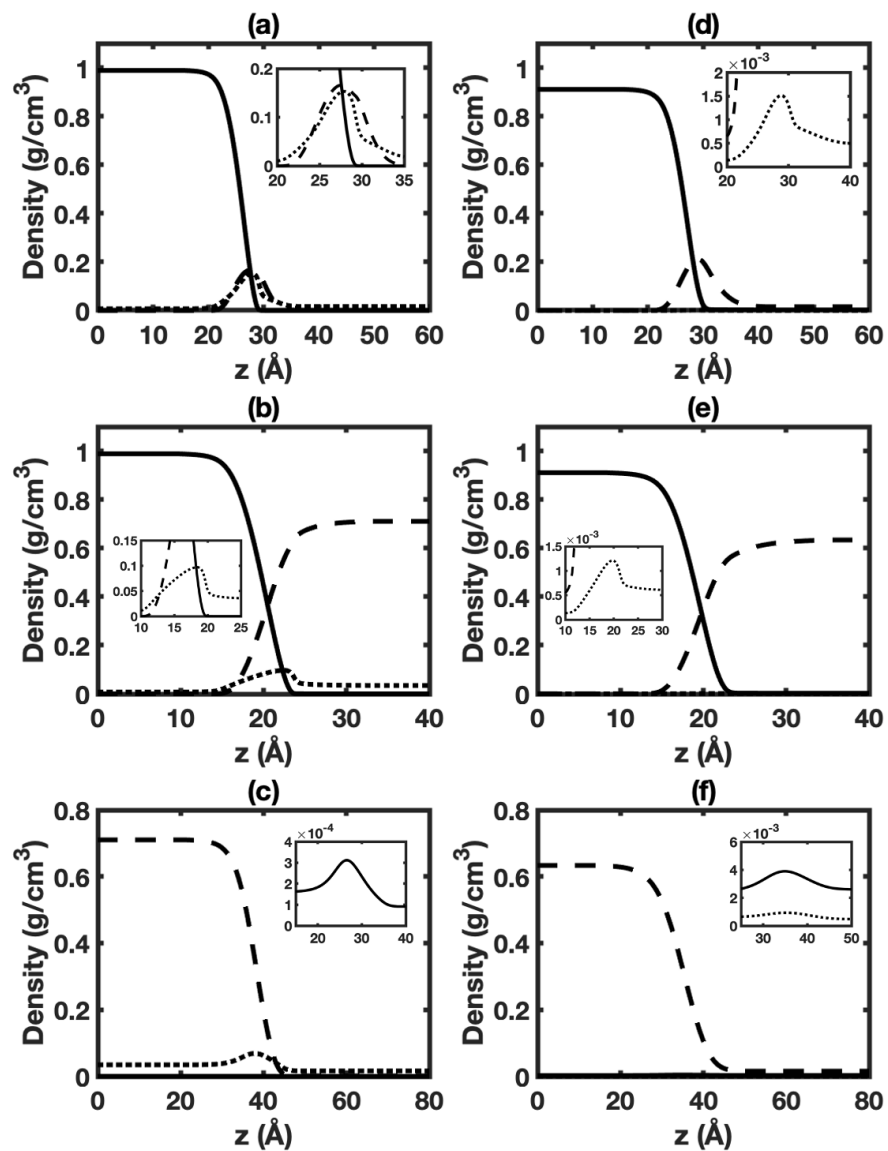


Figure S22: Same as Fig. 5, but at 1 MPa.

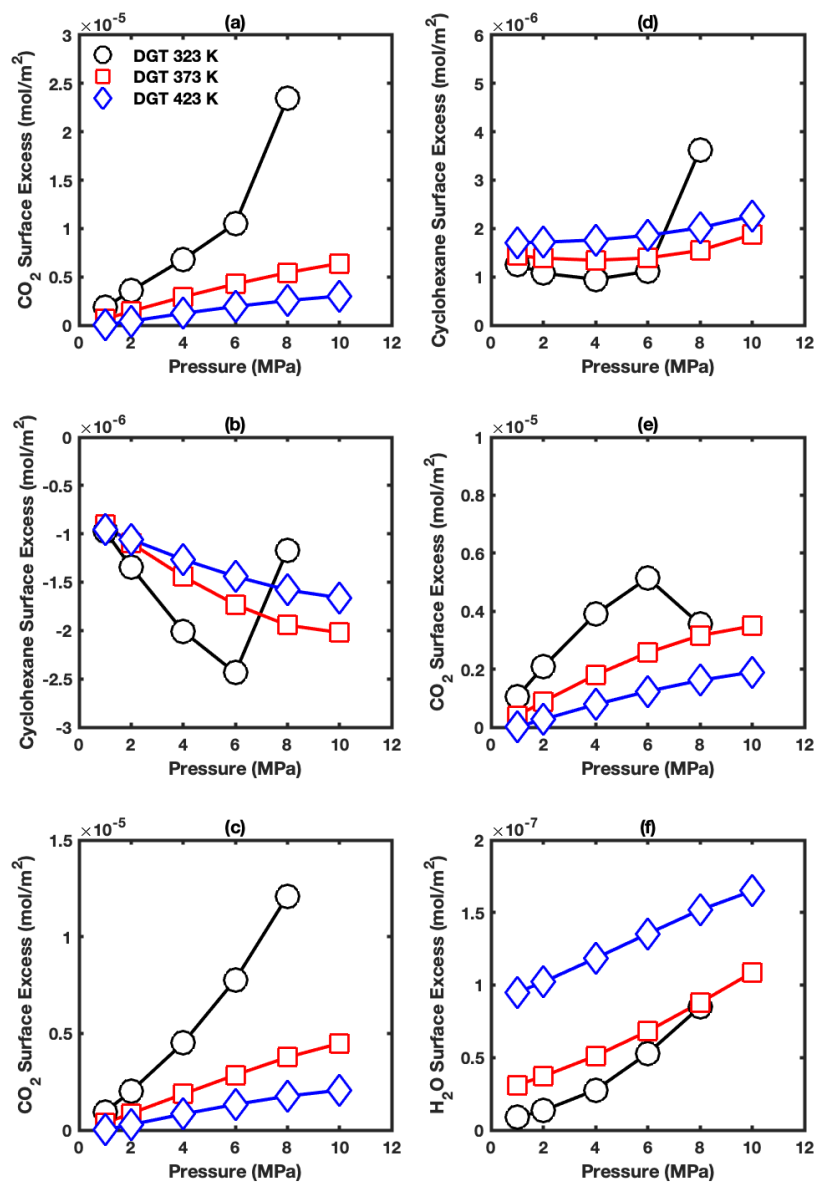


Figure S23: Pressure dependence of component surface excess in $\text{H}_2\text{O}+\text{CO}_2+\text{cyclohexane}$ three-phase system: (a,d) interface of aqueous phase +vapor phase (top panels); (b,e) interface of aqueous phase+cyclohexane-rich phase (middle panels); (c,f) interface of cyclohexane-rich phase+vapor phase (bottom panels).

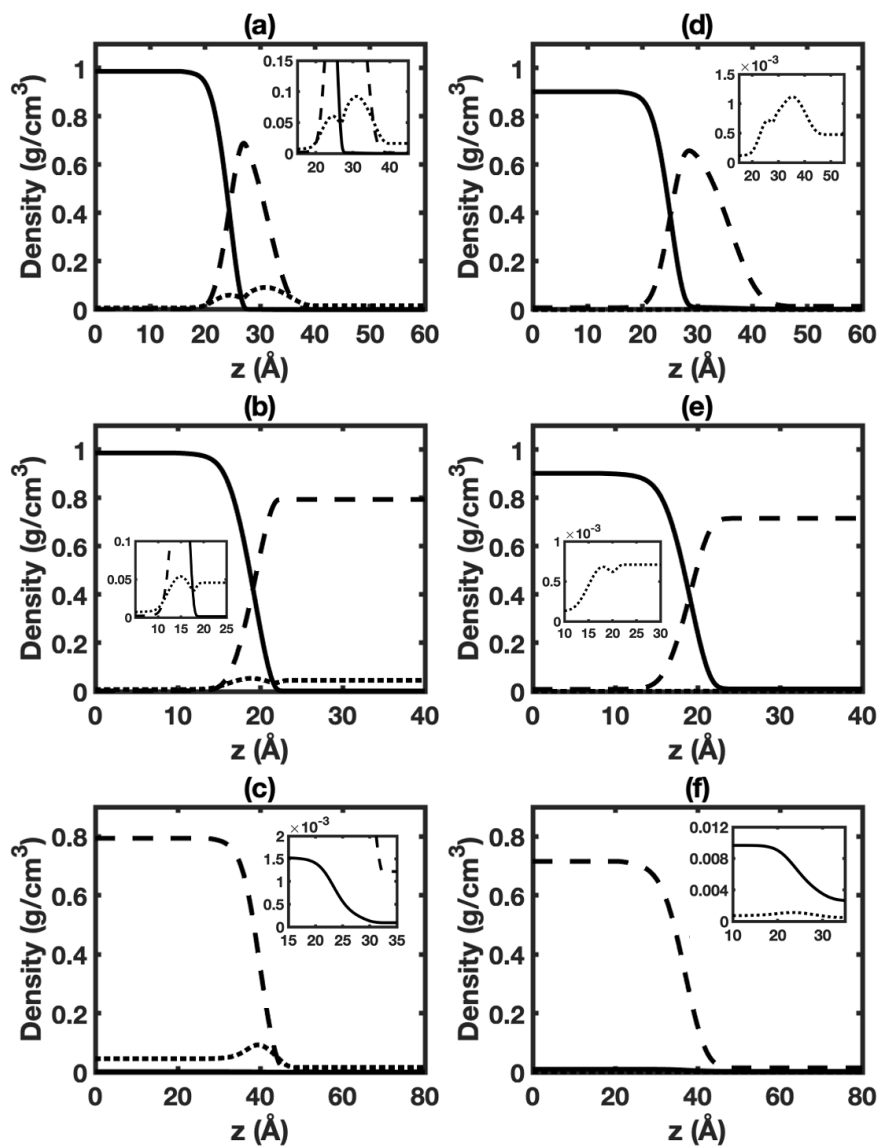


Figure S24: Same as Fig. 7, but at 1 MPa.

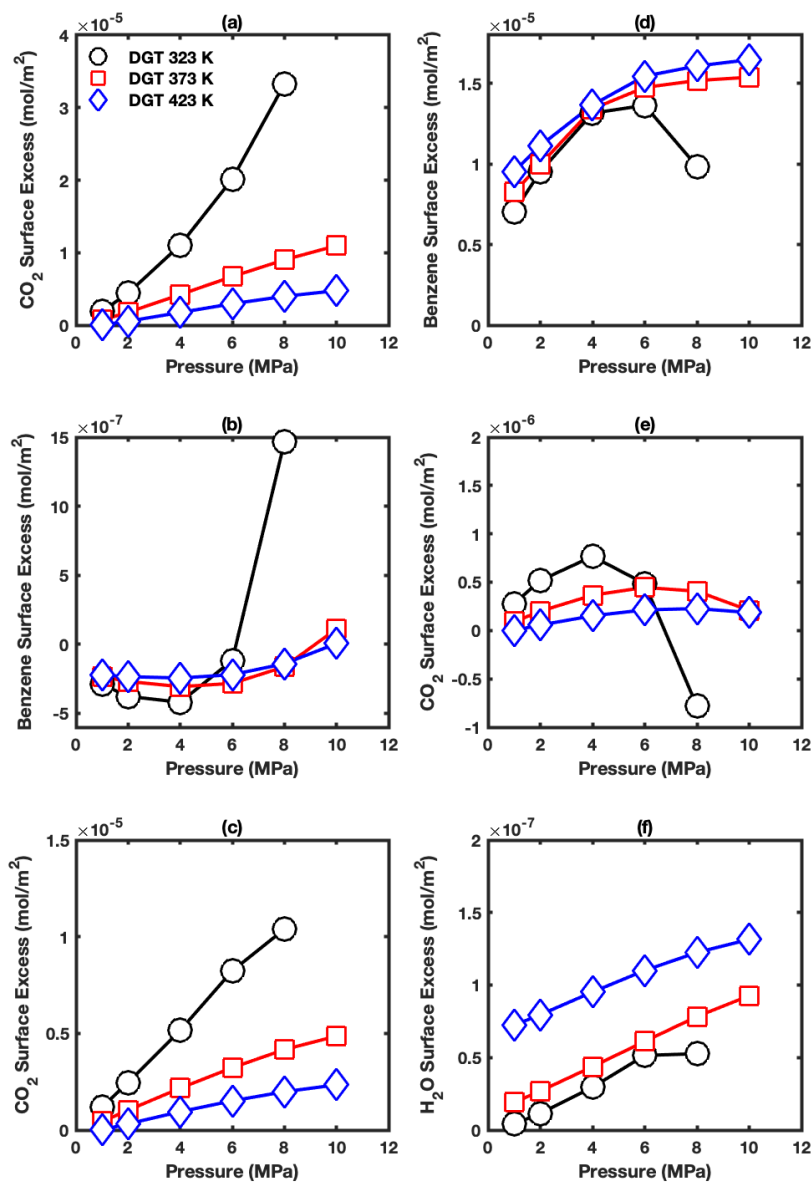


Figure S25: Pressure dependence of component surface excess in $\text{H}_2\text{O}+\text{CO}_2+\text{benzene}$ three-phase system: (a,d) interface of aqueous phase +vapor phase (top panels); (b,e) interface of aqueous phase+benzene-rich phase (middle panels); (c,f) interface of benzene-rich phase+vapor phase (bottom panels).

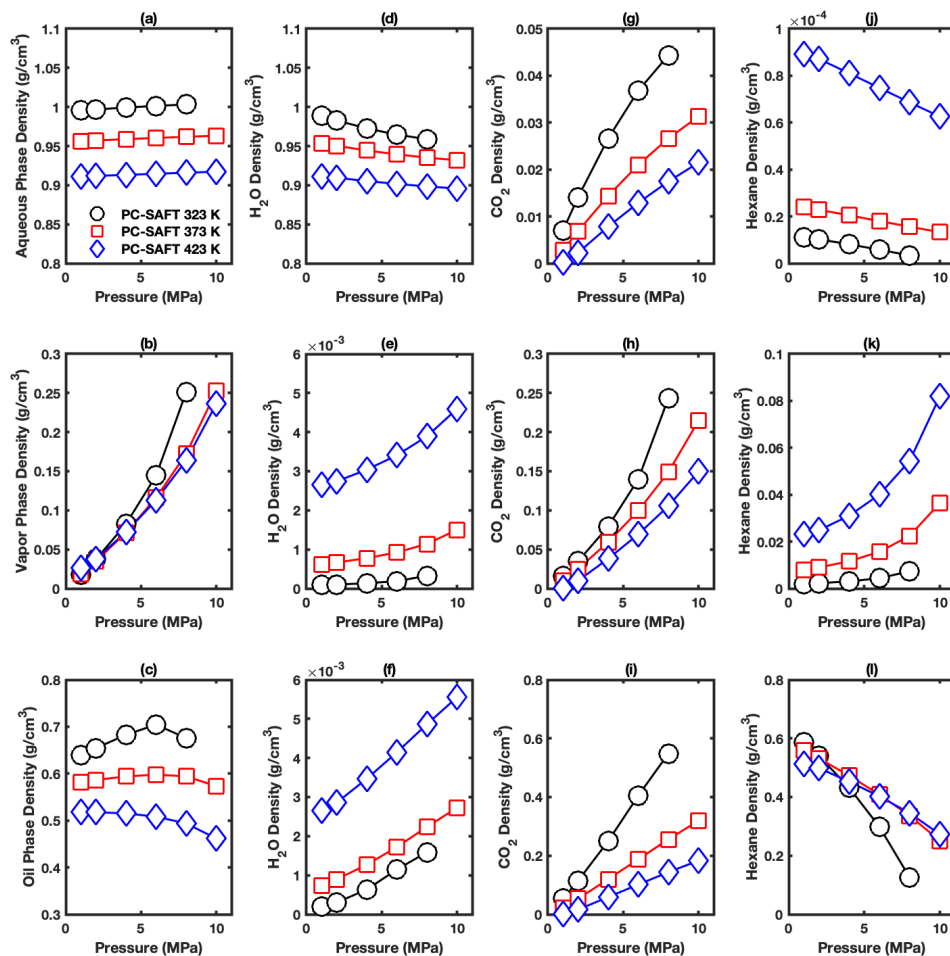


Figure S26: Densities in H₂O+CO₂+hexane three-phase system. Top panels give densities in aqueous phase. Middle panels give densities in vapor phase. Bottom panels give densities in oil phase.

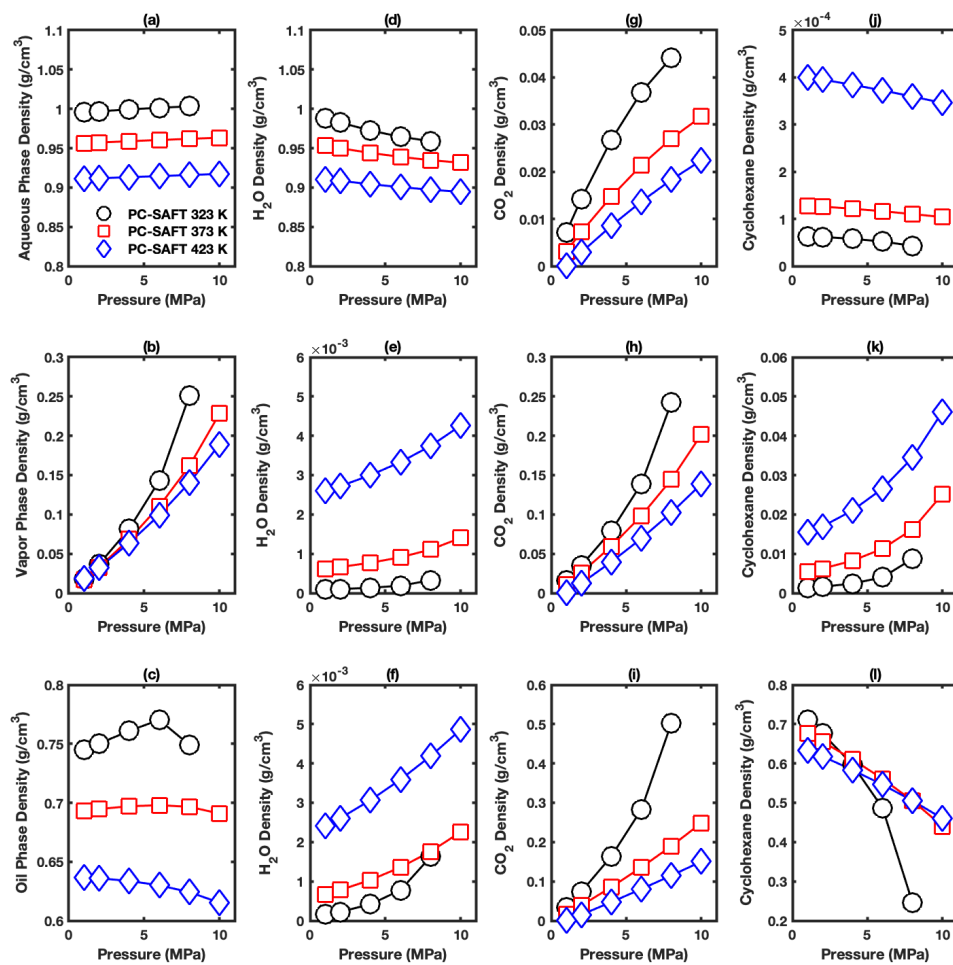


Figure S27: Densities in H₂O+CO₂+cyclohexane three-phase system. Top panels give densities in aqueous phase. Middle panels give densities in vapor phase. Bottom panels give densities in oil phase.

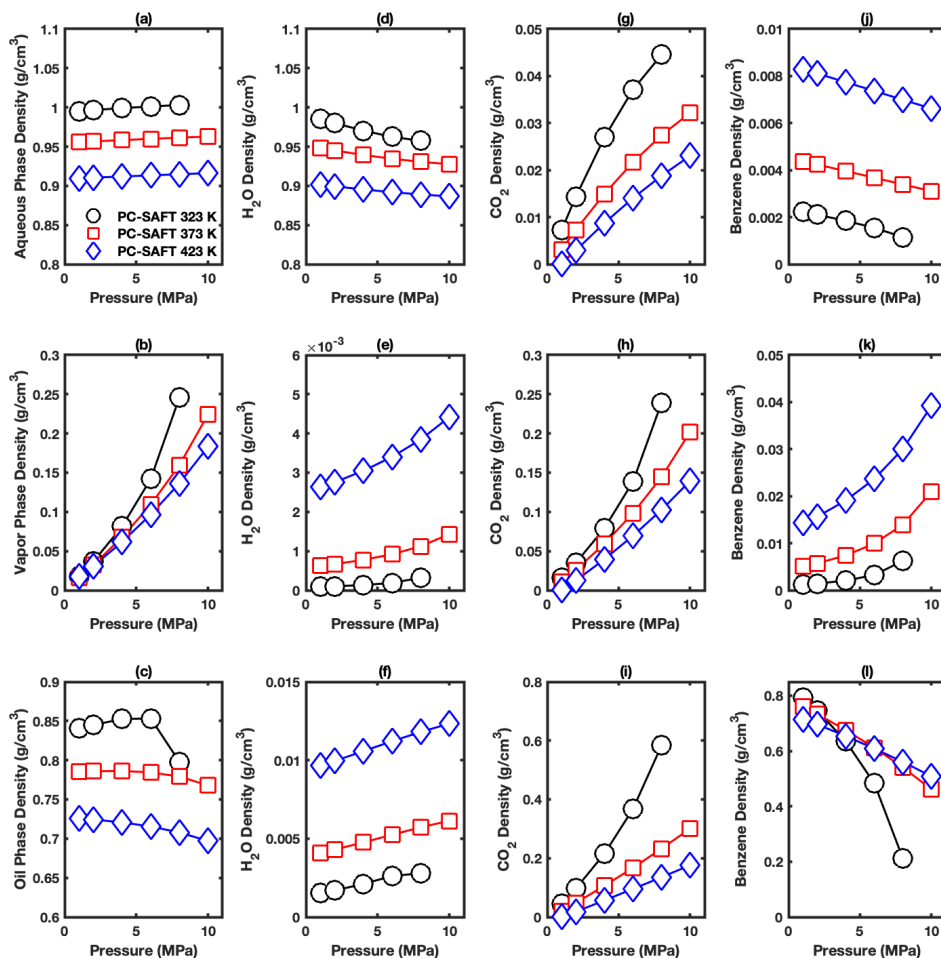


Figure S28: Densities in H₂O+CO₂+benzene three-phase system. Top panels give densities in aqueous phase. Middle panels give densities in vapor phase. Bottom panels give densities in oil phase.

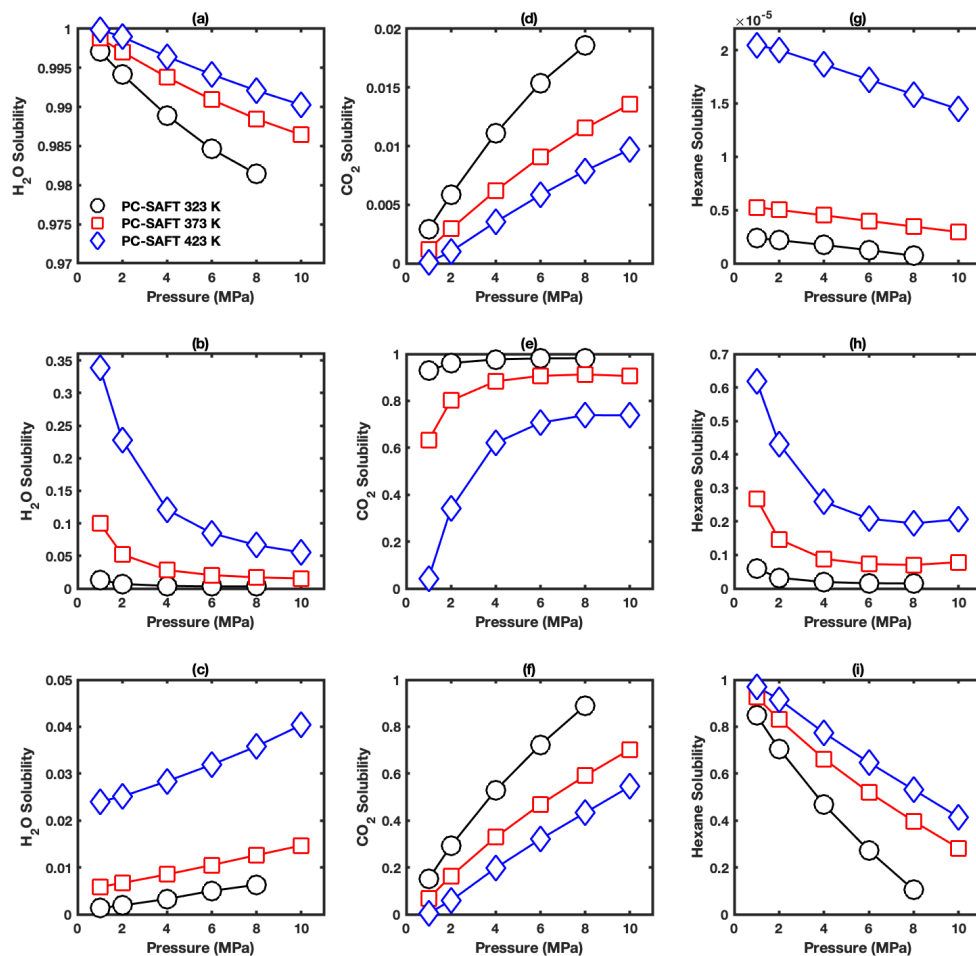


Figure S29: Solubilities in $\text{H}_2\text{O}+\text{CO}_2+\text{hexane}$ three-phase system. Top panels give solubilities in aqueous phase. Middle panels give solubilities in vapor phase. Bottom panels give solubilities in oil phase.

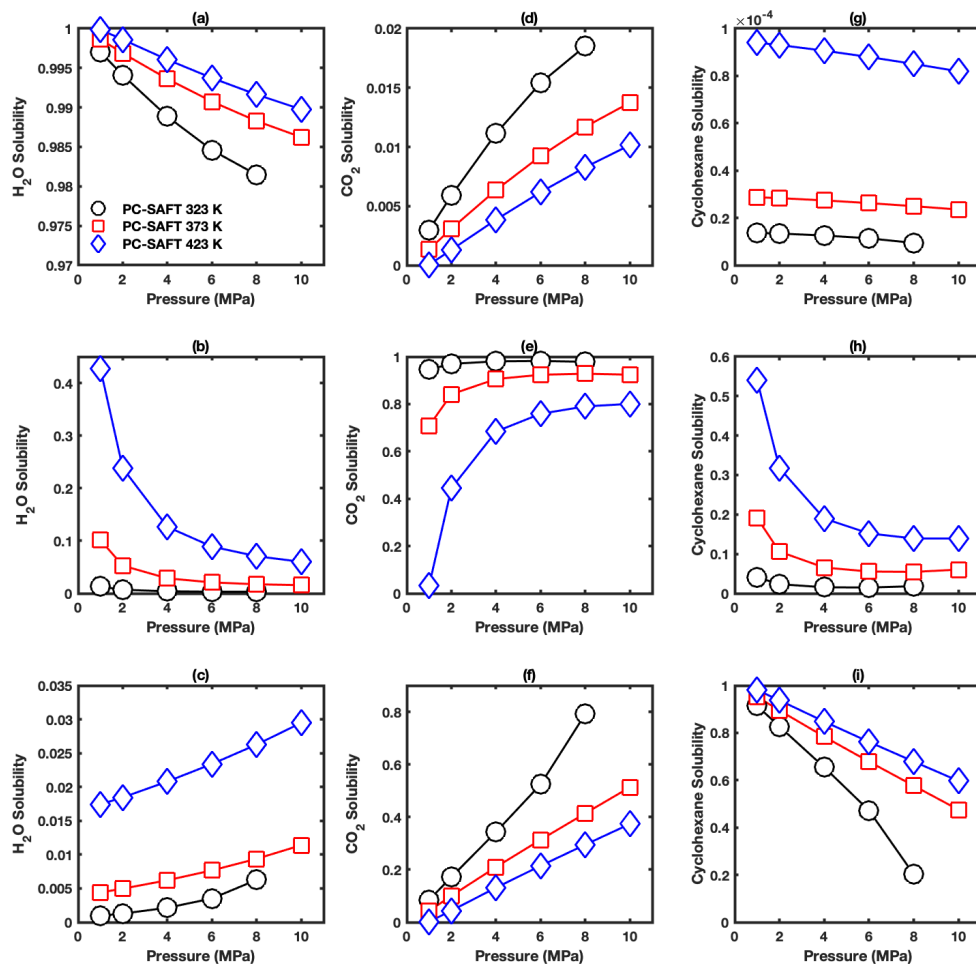


Figure S30: Solubilities in $\text{H}_2\text{O}+\text{CO}_2+\text{cyclohexane}$ three-phase system. Top panels give solubilities in aqueous phase. Middle panels give solubilities in vapor phase. Bottom panels give solubilities in oil phase.

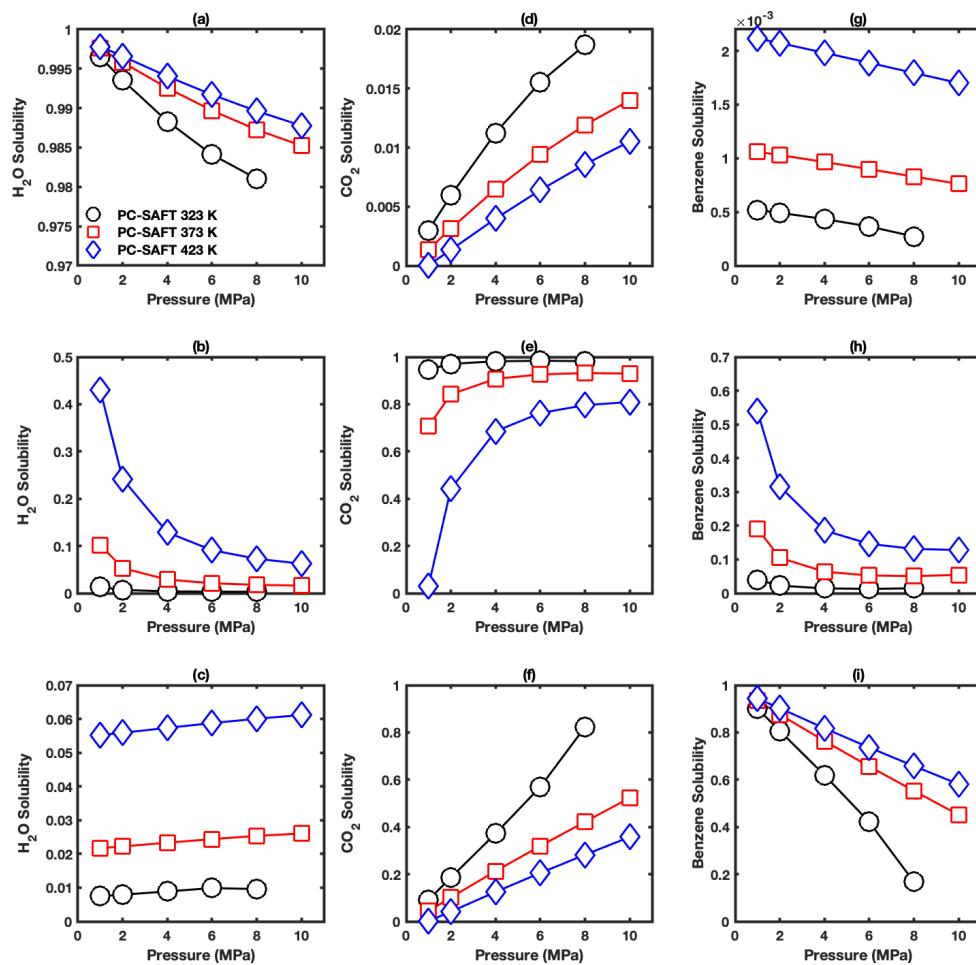


Figure S31: Solubilities in $\text{H}_2\text{O}+\text{CO}_2+\text{benzene}$ three-phase system. Top panels give solubilities in aqueous phase. Middle panels give solubilities in vapor phase. Bottom panels give solubilities in oil phase.