Supporting Information for “Molecular Dynamics Simulation Study of Carbon Dioxide, Methane, and Their Mixture in the Presence of Brine”

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**Figure S1:** Temperature dependence of the surface tension of methane as computed from the MD simulations (symbols) and the corresponding experimental data (NIST Chemistry WebBook).
Figure S2: Density of CO$_2$ at 308.15 K and different pressures as computed from the MD simulations (symbols) and the corresponding experimental data (NIST Chemistry WebBook). The dotted line is the critical pressure (about 7.38 MPa).
Figure S3: Temperature dependence of the surface tension of water as computed from the MD simulations (symbols) and the corresponding experimental data (Vargaftik et al., 1983).
Figure S4: Temperature dependence of IFT for the (a) CH₄–water system and the CH₄–brine system: (b) 5 wt% NaCl and (c) 10 wt% NaCl, as computed from the MD simulations. Lines are a guide to the eyes.
Figure S5: IFT dependence on salt concentration (molality) for the CH$_4$–brine system as computed from the MD simulations: (a) 311, (b) 373, (c) 423, and (d) 473 K. Lines are a guide to the eyes.
Figure S6: Temperature dependence of IFT for the (a) CO$_2$–water system and the CO$_2$–brine system: (b) 5 wt% NaCl and (c) 10 wt% NaCl, as computed from the MD simulations. Lines are a guide to the eyes.
**Figure S7:** IFT dependence on salt concentration (molality) for the CO$_2$–brine system as computed from the MD simulations: (a) 333, (b) 344, (c) 373, and (d) 423 K. Lines are a guide to the eyes.
Figure S8: IFT dependence on mole fraction of CO$_2$ $x_{\text{CO}_2}$ for the CO$_2$–CH$_4$–water (left panels) system and the CO$_2$–CH$_4$–brine (right panels) system with 10 wt% NaCl. Shown are the simulation results at 348 (top panels) and 398 K (bottom panels). Lines are a guide to the eyes.
Figure S9: Same as in Fig. 8, but at 348 K and 7 MPa.
**Figure S10:** Same as in Fig. 8, but at 348 K and 25 MPa.
Figure S11: Same as in Fig. 8, but at 398 K and 7 MPa.
Figure S12: Same as in Fig. 8, but at 398 K and 16 MPa.
**Figure S13:** Same as in Fig. 8, but at 398 K and 25 MPa.
Figure S14: The mole fraction of methane in the water-rich phase versus the mole fraction of CO₂ in the methane or CO₂-rich phases for the CO₂—CH₄—water (left panels) system and the CO₂—CH₄—brine (right panels) system with 10 wt% NaCl. Shown are the simulation results at 348 (top panels) and 398 K (bottom panels).
**Figure S15:** The mole fraction of CO₂ in the water-rich phase versus the mole fraction of CO₂ in the methane or CO₂-rich phases for the CO₂–CH₄–water (left panels) system and the CO₂–CH₄–brine (right panels) system with 10 wt% NaCl. Shown are the simulation results at 348 (top panels) and 398 K (bottom panels).
Figure S16: The mole fraction of H$_2$O in the methane or CO$_2$-rich phases versus the mole fraction of CO$_2$ in the methane or CO$_2$-rich phases for the CO$_2$–CH$_4$–water (left panels) system and the CO$_2$–CH$_4$–brine (right panels) system with 10 wt% NaCl. Shown are the simulation results at 348 (top panels) and 398 K (bottom panels).
Figure S17: Equilibrium distributions of orientations for the water dipoles, H-H vectors of the water molecules, and head-to-tail vectors of the CO$_2$ molecules (from top to bottom, respectively) relative to the axis perpendicular to the interface at 348 K and 7 MPa. Shown are the simulation results for the CO$_2$−CH$_4$−water (left panels) system and the CO$_2$−CH$_4$−brine (right panels) system with 10 wt% NaCl. The mole fraction of CO$_2$ $x_{CO_2} \approx 0.6$. Bright regions correspond to high probabilities of orientation angles.
Figure S18: Same as in Fig. S17, but at 348 K and 16 MPa.
Figure S19: Same as in Fig. S17, but at 348 K and 25 MPa.
Figure S20: Same as in Fig. S17, but at 398 K and 7 MPa.
Figure S21: Same as in Fig. S17, but at 398 K and 16 MPa.
Figure S22: Same as in Fig. S17, but at 398 K and 25 MPa.
Figure S23: Effect of the choice of water model on the pressure dependence of IFT for the CO$_2$–CH$_4$–water system at 423 K. Shown are the results obtained from the MD simulations (symbols) and the corresponding experimental data (Kashefi et al., 2016; Pereira et al., 2016).