Supercritical water-carbon dioxide fluids through the transition zone

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Recent discoveries of water and carbon dioxide in minerals originating from the deep mantle have shown that the water and carbon cycle extends deep into the mantle. Thermodynamic properties in the CO_2-H_2O system have been intensively studied at low pressures. At high pressures, experimental and computational approaches have provided equation of state up to 11GPa. It is very difficult to measure volumes of fluid systems experimentally, so we are using first-principles simulations to constrain the fluid properties. We performed first principles molecular dynamics (FPMD) on 4 isotherms (1000-2500K) up to pressures of 30 GPa. We constructed a pressure-volume-temperature-composition (PVTX) equation of state (EOS) which describes the properties of C-bearing supercritical fluids up to lower mantle conditions. We find good agreement with fluid inclusion experiments at pressures greater than 1GPa. The excess volumes of CO_2-rich mixtures decrease with pressure, finding more ideal mixing at high pressures. CO_2-poor fluids mix ideally at upper mantle conditions. Our equation of state is accurate from 4 to 30GPa, and complement to the existing dataset, extending the thermodynamic data to deep mantle conditions.

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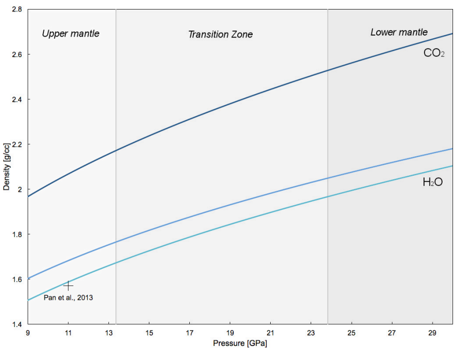

Figure 1: Densities of 3 supercritical fluids at 1000K. H_2O, CO_2 and an aqueous fluid containing 0.14 mol% CO_2 are shown.