



## **Carbon Dioxide – rock interaction: from molecular observations to theorised interactions in fluid-rock systems**

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Current global warming theories have produced some benefits: among them, detailed studies on CO<sub>2</sub> and its properties, possible applications and perspectives. Starting from its use as a “green solvent” (for instance in decaffeination process), to enhance system in oil recovery, to capture and storage enough amount of CO<sub>2</sub> in geological horizon. So, a great debate is centred around this molecule.

One More useful research in natural horizon studies is its theorised use in Enhanced Geothermal Systems with CO<sub>2</sub> as the only working fluid. In any case, the CO<sub>2</sub> characteristics should be deeply understood, before injecting a molecule prone to change easily its aggregation state at relatively shallow depth.

CO<sub>2</sub> Rock interaction becomes therefore a focal point in approaching research sectors linked in some manner to natural or induced presence of carbon dioxide in geological horizons. Possible chemical interactions between fluids and solids have always been a central topic in defining evolution of the system as a whole in terms of dissolutions, reactions, secondary mineral formation and, in case of whichever plant, scaling.

Questions arise in case of presence of CO<sub>2</sub> with host rocks. Chemical and molecular properties are strategic. CO<sub>2</sub> Rock interactions are based on eventual solubility capability of pure liquid and supercritical CO<sub>2</sub> seeking and eventually quantifying its polar and/or ionic solvent capabilities.

Single molecule at STP condition is linear, with central carbon atom and oxygen atoms at opposite site on a straight line with a planar angle. It has a quadrupolar moment due to the electronegativity difference between carbon and oxygen. As soon as CO<sub>2</sub> forms bond with water, it deforms even at atmospheric pressure, assuming an induced dipole moment with a value around 0.02 Debye. Hydrated CO<sub>2</sub> forms a hydrophilic bond; it deforms with an angle of 178 degrees. Pure CO<sub>2</sub> forms self aggregates. In the simplest case a dimer, with two molecules of CO<sub>2</sub> exerting mutual attraction and forming at a first impact a structure defined parallel or slipped parallel or a more stable T shaped. As soon as pressure is applied, density changes and appears a stable (induced) dipole moment 0.22 Debye: phase changes and CO<sub>2</sub> dipole moment reaches 0.85 Debye dipole moment. Pure CO<sub>2</sub>, here the only liquid phase, assumes Lewis acid/base properties. Polar solvent properties seem to be real, and some experiments have observed this characteristics.

This stated, present work try to show computer aided simulation in chemical and physical evolution of a portion of rock with liquid and supercritical CO<sub>2</sub>, with and without water, in granite and oceanic basalt formations.