A numerical simulation of a mineral precipitation/dissolution by a rapid decompression of brine

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The dielectric constant is a key parameter characterizing chemical properties of solvents. The apparent constants of 1 molal NaCl solutions at P = 50-400 MPa and T = 25-500°C have been preliminary formulated from previous experimental data of quartz solubilities in H_2O -NaCl solutions as:

 $\varepsilon_{\rm b} / \varepsilon_{\rm w} = a / (2 \pi b)^{0.5} \exp(-(T - c)^2 / (2 b)) + d,$

where, $\varepsilon_{\rm b}$ is the constant of the 1 molal NaCl solution, $\varepsilon_{\rm w}$ is that of water derived by SUPCRT92, π represents the ratio of the circumference of a circle to its diameter, T is a temperature in Celsius, the parameter a depends on a pressure (P in MPa) as a = -0.9 * P + 420, and b, c and d are the constants as 13000, 300 and 0.8, respectively.

On the other hand, a difference in chemical potentials of a jth solute ($\Delta \mu_{j}^{\circ}$) in the solution and water may be expressed as:

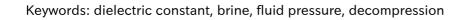
$$\Delta \mu_{j}^{o} = \omega_{j} (1/\varepsilon_{b} - 1/\varepsilon_{w}),$$

where, ω_j is the Born coefficient of the solute. Hence, mineral solubilities in the solutions may differ greatly from those in water at around 300°C, and the differences may commonly be larger as the pressures lower.

Seismic faulting may cause rapid fracturing around the fault planes, hence fluid pressures in the fractures and pores may decrease rapidly. By taking account of the above P and T dependencies of the apparent dielectric constants of the 1 molal NaCl solutions, quartz and calcite precipitations/dissolutions from the solutions and water by in situ decompressions from lithostatic to hydrostatic pressures have been simulated under magnetite-hematite oxygen buffers. The lithostatic P-T relation is assumed with a geothermal gradient of 25°C/km and a rock density of 2.8 g/cc, while the hydrostatic P-T curve is obtained by accumulation of water columns downwards with water densities at given P-T conditions provided by NIST.

When the fluids of temperatures 200-450°C (at depths of 7-17 km) decompress isenthalpically from lithostatic (196-476 MPa) to hydrostatic (66-145 MPa) pressures, the temperatures increase about 20°C at the all depths. However, irrespective of the temperature increases, quartz precipitates from the solutions and water in the all simulated isenthalpic decompressions. For example, the amounts of quartz precipitations (mole/kg-water) from the solutions and water at 17 km depth from lithostatic (476 MPa-450°C) to hydrostatic (145 MPa-469°C) conditions are 0.0048 and 0.0061, respectively, while those at 7 km depth (from 196 MPa-200°C to 66 Ma-218°C) are 0.00019 and 0.00014, respectively. The amounts of quartz precipitations from the solutions and water increase with the depths. The amounts of calcite coprecipitating with quartz from water by isenthalpic decompressions also increase monotonically with the depth, while the amount from the 1 molal NaCl solutions is smallest at around 15 km (350°C). When the solution is equilibrated with calcite only, it dissolves at the depths 11 -

15 km (300-400°C) by the decompressions. The great difference in precipitation/dissolution amounts of calcite from water and the solution is due to the large difference in the dielectric constants of water and the solution at around 300° C.



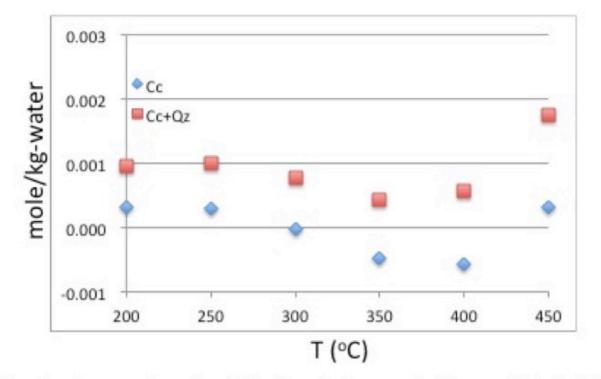


Fig. 1 Amounts of calcite (mole/kg-water) precipitated (+)/ dissolved (-) from 1 molal NaCl solutions equilibrated with only calcite (diamond) and with quartz (square) during isenthalpic decompressions.