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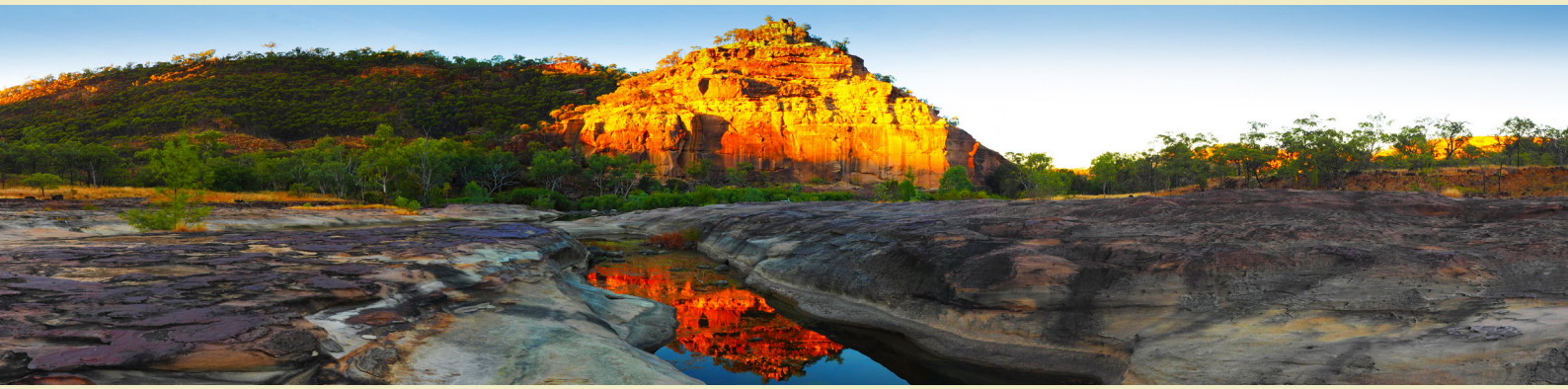

Modelling of hydrothermal fluid compositions in the crust and upper mantle

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Carbon-oxygen-hydrogen (COH) fluids are integral to the formation of many hydrothermal ore deposits (including orogenic gold, graphite), and diamond. Typically, a crustal/upper mantle COH fluid comprises H_2O, CO_2, CH_4, H_2, CO, C_2H_6, and O_2.

Crustal and upper mantle fluid compositions are constrained by pressure, temperature and redox state, and can be calculated if: (1) A reliable equation of state for fluid mixtures is available for the relevant pressure-temperature conditions is available for the calculation of fugacity coefficients; (2) Reliable thermodynamic variables including enthalpy, entropy and isobaric heat capacity can be obtained.

Here, we used the equation of state by Zhang and Duan (2009) in conjunction with the NIST reference dataset to develop a user-friendly Excel spread sheet that allows the calculation of fluid compositions for a pressure-temperature range of > 0.5 kbar and 300-1500°C, respectively. Data manipulation and modelling was achieved with a combination of VBA, Python and SQL scripting and allowed us to validate the model calculations in the Excel spread sheet.

Reference

Zhang, C. and Duan, Z. (2009). A model for C-O-H fluid in the Earth's mantle. Geochimica et Cosmochimica Acta 73, 2089-2102.