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Model-derived uncertainties in the calculation of geological phase equilibria

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Phase equilibrium modelling offers a welcome window onto rock-forming processes. It underpins the principles of geothermobarometry, which today is commonly carried out via pseudosection calculations in software such as THERMOCALC and Perple_X. Increasingly, phase equilibrium modelling is combined with complementary approaches such as diffusion or geodynamical calculations, in order to simulate Earth processes.

However, as anyone with experience of pseudosection calculations will know, it is not always easy to make sense of a rock through phase equilibrium modelling. Problems may relate to: (1) in what way the assumption of thermodynamic equilibrium may, or may not, be applied; (2) uncertainties in compositional analysis; and (3) uncertainties in the composition-dependent equations of state (*x*-eos). The *x*-eos are the building blocks of the modelling – one *x*-eos is needed to represent each of the mineral and fluid phases in the calculation.

Of the problems listed above, (3) is the most opaque for the user. In this talk I will discuss the uncertainties associated with the *x*-eos, and the implications of those uncertainties for thermobarometry and the simulation of Earth processes. I will describe two tools, currently in development, for investigating *x*-eos-derived uncertainty in thermobarometry.