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Adapting phase equilibria modelling to crustal and planetary scale problems

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Modern quantitative phase equilibria modelling techniques utilizing internally consistent datasets and activity-composition models have been successfully applied to a number of problems in metamorphic geology from hand sample to outcrop scale. Attesting to this the term “phase equilibria” appears in 1 548 articles in the Journal of Metamorphic Geology and one third of those are within the last 10 years. These techniques traditionally proceed either through the manual solution of non-linear equations or by a more automated Gibbs free energy minimization approach. However in order for these techniques to be scaled up to deal with crustal or planetary scale problems a number of hurdles still need to be overcome.

Spatial dimensions in a crustal or planetary model are estimated by grids with modelling conducted on individual cells. This allows processes within cells to effect chemical change to partner cells and thereby approximate open or conditionally open systems. Compositional constraints to the chemical system such as oxygen fugacity are pressure and temperature dependent therefore in order to model a planet wide set of conditions oxygen fugacity buffers are enabled that are dependent on the pressures and temperature of the individual grid cells. Stratigraphic layering is introduced by automating the procedure for setting the initial composition of cells and dependence relations determine the hierarchy of compositional change induced within crustal columns. Phase manipulations such as fluid, melt or crystal addition or extraction are defined by mechanistic parameters that simulate boundary conditions for example melt accumulation thresholds, fluid porosity threshold, rheological lockup conditions etc. Since certain key chemical parameters used in identifying crustal processes such as trace element ratios cannot be traditionally modelled due to their absence from the internally consistent thermodynamic datasets new methods of component approximation are introduced following the methods of trace element partitioning and accessory phase saturation for supersolidus systems.

Finally the increased complexity and number of calculations required to scale up phase equilibria modelling systems to the crustal or planetary scale provides an increased computational challenge therefore new potential strategies are explored for the optimizing of calculation load via parallel processing.