Computational thermodynamics: towards an improved Gibbs minimization tool for geodynamic modelling

Nicolas Riel$^1$, Boris Kaus$^1$, Nicolas Berlie$^1$, Lisa Rummel$^2$, and Eleanor Green$^3$

$^1$Institute of Geosciences, Johannes Gutenberg University Mainz, J.-J.-Becher-Weg 21, D-55128, Mainz, Germany
$^2$Institute of Geosciences and Natural Resources (BGR), Hannover, Germany
$^3$Science division, Melbourne University, Melbourne, 04, 416a, McCoy Building/Earth Sciences, Parkville, Australia

In the last decade, the development of numerical geodynamic tools helped the geoscience community to explore thermo-mechanical processes at play during plate tectonics. Yet, the high computational cost of thermodynamic calculations hampers our ability to quantify multi-phase systems in which the interplay between plate-tectonics and phase transformations leads to magmatism. Here we use the 'igneous set' of HPx-eos (thermodynamic models for minerals and geological fluids that are based on the Holland & Powell dataset and defined in the THERMOCALC software) to calculate stable phase equilibria in the system K$_2$O–Na$_2$O–CaO–FeO–MgO–Al$_2$O$_3$–SiO$_2$–H$_2$O–TiO$_2$–Fe$_2$O$_3$–Cr$_2$O$_3$ (KNCFMASHTOCr). The calculation is performed by Gibbs free energy minimization at prescribed pressure, temperature and bulk-rock composition and is achieved in two steps. First, we employ a levelling method (iterative change of base) to reduce the number of potential stable phases. Then, the composition and proportions of stable phases at equilibrium are determined using several constrained optimization methods. We explore the computational efficiency of linear programming (e.g., Simplex), Gradient-based (e.g., SLSPQ) and Hessian-based (e.g., Newton-Raphson) methods. The accuracy and performance of tested methods are compared, and applications to geodynamic modelling are discussed.