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# Accessory phase saturation and trace element partitioning in combination with compositionally flexible phase equilibrium modelling in Rcrust: A new tool for igneous petrology.

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Magma formation and evolution may involve multiple processes that result in change in the chemistry of a rock system. Most notable of these are segregation from residuum, crystal entrainment, wall rock assimilation, magma mixing and fractional crystallization. Phase assemblage change due to these processes can readily be modelled using the Rcrust phase equilibria modelling tool which has been developed using a unique path dependent algorithm to allow compositional change [1,2].

Understanding the behaviour of the accessory phases, apatite, monazite and zircon are important in igneous and metamorphic petrology, particularly due to their role as geochronometers and thermochronometers. Current thermodynamic databases and liquid- and solid-solution phase activity-composition models cannot accomodate minor and trace elements as chemical components in modelled systems. For the phases of interest above, phase saturation routines have been developed using the solubility of P and Zr within melt, coupled with the LREE budget, to calculate when and in what proportion monazite, apatite and zircon will form part of the mineral assemblage. Finally, activity distribution coefficients have been incorporated to allow Rcrust to partition trace elements between melt and the stable phases.

This novel approach allows trace elements to be forward modelled and compared to observations from natural and experimental results. Initial results highlight the importance of major element components that also contribute to accessory phase formation such as calcium in apatite (which can accommodate a non-trivial quantity of the available calcium) and the resultant effect on phase equilibria of major phases. By modelling both major and accessory phases we provide constraints on the formation and crystallisation of crustal magmas which has important implications on geothermobarometry and thermochronology in the crust.

[1] Mayne et al. (2016) *J. Met. Geol*. **34**(7), 663-682. https://doi.org/10.1111/jmg.12199

[2] Mayne et al. (2020) *Geol. Soc. Spec. Publ.* **491**(1), 209-221. https://doi.org/10.1144/SP491-2018-85