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Tracking the Archean upper mantle oxygen fugacity using mafic-ultramafic rocks geochemistry- a machine learning-based approach

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The redox condition of the early terrestrial atmosphere is a matter of widespread debate. It is directly linked to the redox state of the upper mantle through volatile exchange between the two reservoirs [1]. Basalts and komatiites, which constitute major components of the Archean mafic crust, can mirror the oxygen fugacity (fO_2) of their mantle source. Here we use the major oxides chemistry of basaltic liquids (n=616) from experimental studies with well-constrained pressure-temperature-fO_2 conditions and apply three robust machine learning models-random forest, XGBoost, and LightGBM regression models, to calibrate the relationship between basaltic melt composition-pressure-temperature, and fO_2. We tested these three models over a subset of the experimental dataset and obtained good predictive performance (NRMSE of 0.09, 0.1, 0.11, and R^2 scores of 0.8, 0.73, 0.72, respectively). We further implement SHAP algorithm to these models to determine the parameters with the strongest influence (i.e., FeO^T, MgO, temperature, TiO_2, K_2O of melt) on the melt fO_2 estimation. From a global compilation of 3.8-2.5 Ga Archean basaltic rocks (n=1091), we estimated the composition of their primitive parental melts, as well as the P-T conditions under which they formed using the “Fractionate-PT” program [2]. The outcomes combined with our trained models are then used to assess the melt fO_2 vis-à-vis the source mantle redox condition prevailing then. Our results indicate a slight increase in the melt fO_2 (~0.5 log units) between 3.8 Ga and 3.5 Ga, after which it remained constant until 2.6 Ga, followed by slight increase in melt fO_2 at the end of Neoarchean. The moderate increase in mantle redox conditions in the Eoarchean is possibly due to enhanced supracrustal recycling, which remained more or less constant till the Neoarchean. Together with detrital zircon Hf-O isotope evidence of transition in Archean granitoids in the 3.60-3.85 Ga time-period [3], we speculate that this change in fO_2 of mantle-derived melt may reflect the initiation of subduction that facilitated increased supracrustal recycling in the Eoarchean.

[1] Kadoya et al. (2020), Nat. Commun. **11**, 2774. [2] Lee et al. (2009), Earth Planet. Sci. Lett. **279**, 20–33. [3] Drabon et al. (2022), AGU Adv. **3**, e2021AV000520.