Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.36235

MELTS+DEW thermodynamic framework supporting modeling of elemental partitioning between magmas and CO_2-rich aqueous fluids

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We have previously reported [1,2] on the construction and calibration of a thermodynamic modeling framework that couples MELTS [3] with the Deep Earth Water (DEW) model [4], which extends the former to permit modeling of elemental partitioning between magmas and aqueous fluids. This work saw the addition and calibration of Cl, F and S to the silicate liquid thermodynamic model in MELTS and the development of software to facilitate computational coupling of the modeling frameworks. Lacking from our previous work is extension of the MELTS+DEW thermodynamic framework to CO_2-rich aqueous fluids. While an H_2O-CO_2 molecular fluid model has previously been incorporated within MELTS [6], partitioning of other elements to the fluid cannot be readily extended with this methodology. To address this deficiency, we have developed an approach [6] for extending the DEW model to account for CO_2-rich solvents. This approach involves recasting rational activity coefficients calculated from models presented by [7] and [8] into an Henrian (aqueous) standard state/activity formulation compatible with the extended-HKF modeling framework [9] underpinning DEW. Calibration of novel activity coefficient expressions for the mixed H_2O-CO_2 electrolyte and compatible extended-HKF standard state properties for CO_2-rich species in the aqueous phase, generates a revised DEW model that permits calculation of the compositions of CO_2-rich aqueous fluids saturated in magmas. Applications to fluid saturation in a broad spectrum of CO_2-bearing magma types are presented, including the effects of additional fugitive magmatic components (e.g. Cl) on the compositions of derived fluids.

[1] https://doi.org/10.7185/gold2023.13890, [2] https://doi.org/10.7185/gold2023.19432, [3] Contrib. Mineral. Petrol. 119:197-212; 169:53, [4] Geochim. Cosmochim. Acta 129:125-45; 254:192-230, [5] https://doi.org/10.1007/s00410-015-1141-8, [6] https://doi.org/10.7185/gold2023.20616, [7] Am Mineral. 84, 1319-1332, [8] https://doi.org/10.1016/j.gca.2006.02.009, [9] https://doi.org/10.2475/ajs.288.1.19