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Experimental and numerical constraints on the distribution of volatiles between rocky planet interiors and atmospheres

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Magma worlds, due to their hot, extended atmospheres are readily characterized spectroscopically by ground- and space-based telescopes, such as JWST. These upcoming exoplanet observations will unlock a new pathway for studying the early Earth and possibly the origin of life on both our planet and others. As yet, the lack of direct observations means that the nature and composition of these magma exoplanets' atmospheres are poorly constrained. Because the atmospheres of these planets are thought to be the result of chemical equilibrium with their interiors, their mass and composition are modulated by the solubilities of major gases in the magma. Therefore, we require a theoretical framework, informed by experimental data, to determine how volatile elements partition between the interior and atmosphere for diverse planetary compositions, including the early Earth. However, there is limited experimental data on the solubilities of major atmosphere-forming gases in a range of silicate liquids which may be unlike that of the present-day Earth, including that of Earth's primitive mantle. To fill this gap, we performed new volatile (e.g., H, C, O) solubility experiments on planetary melt analog materials (e.g., peridotitic melts, chondritic meteorite materials) at high temperatures (1400 ℃) using a 1-bar H_2-CO_2 gas-mixing furnace and an aerodynamic laser levitation furnace coupled to an FTIR spectrometer. We incorporate these experimental results into a new Python package (*atmodeller*), which computes chemical equilibrium at the melt-atmosphere interface of rocky worlds. Given a set of planetary parameters (e.g., surface temperature, planetary mass, radius, mantle melt fraction) and initial volatile inventory, *atmodeller* uses experimentally calibrated solubility laws (including those determined from our experiments), together with free energy data for condensed and gas species, to determine how volatiles partition between the atmosphere and interior. Within the H-He-C-N-O-S-Cl system, we investigate a range of plausible atmospheric compositions and the impact of volatile dissolution into the interior for a set of plausible early Earth scenarios and several known hot, rocky exoplanets given current observational constraints from JWST.