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Diversity of rocky planet atmospheres in the H-C-O-N-S-Cl system with interior dissolution

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Given the host of existing and upcoming observations of rocky (exo)planet atmospheres, a quantitative understanding of the key factors that control the nature and composition of atmospheres around these diverse worlds is needed. The speciation of major atmosphere-forming components around molten rocky planets, both within and beyond the solar system, is dictated by their abundances, the equilibrium chemistry between gas species, and their solubilities in the rocky interior. Moreover, as pressure increases at the atmosphere-interior interface, the thermodynamic behaviour of the gas phase diverges from that of the ideal case. Here, we combine these considerations into a new Python package, atmodeller, which is a flexible tool kit for computing the equilibrium conditions at the melt-atmosphere interface. Given a set of planetary parameters (e.g., surface temperature, planetary mass, radius, mantle melt fraction) and an initial volatile budget, atmodeller uses experimentally calibrated solubility laws, together with free energy data for gas species, to determine how volatiles partition between the atmosphere and interior of the planet. This package can be applied widely to rocky planets, from super-Earths to sub-Neptunes with gaseous envelopes. Within the H-C-N-O-S-Cl system, we investigate the diverse range of atmospheric compositions and the impact of volatile dissolution into the interior for a set of known rocky exoplanets (e.g., the TRAPPIST-1 system) based on the current observational constraints from JWST. In addition, we use atmodeller to simulate the effects of volatile solubilities and non-ideal conditions on H2-dominated super-Earth- and sub-Neptune atmospheres (in the H-O-Si system), such as that of the recently observed exoplanet K2-18 b. Atmodeller is a new tool to study rocky (exo)planets, uniquely incorporating equilibrium chemistry, volatile solubilities and gas non-ideality to establish the connection between rocky planet interiors and their atmospheres.