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MAGEC_CHOSN: An integrated thermodynamic framework for modeling C-H-O-S-N distribution in planetary magma oceans

CHENGUANG SUN

The University of Texas at Austin

Presenting Author: csun@jsg.utexas.edu

How C-H-O-S-N distribute in planetary magma oceans is a critical question for understanding the volatile budget, atmosphere evolution, and habitability of rocky planets. Previous considerations of this question often took simplified approaches, such as fewer volatile elements, buffered redox conditions, a chemically isolated core, and ideal behaviors of vapor species at elevated pressure. As indicated by crustal magmatic systems on Earth [1], gas-melt interactions are unlikely controlled by certain redox buffers but instead can be strongly affected by the chemical and redox equilibria of multi-component volatiles in the gas and melt. Decoupling the core chemically from the magma ocean and atmosphere is likely a valid assumption for late-stage magma ocean solidification but may not be applicable to the early magma ocean associated with core formation. These complexities are non-trivial problems and may cause chemical differentiation that have been overlooked before. Based on the MAGEC code of [1] for C-H-O-S distribution in crustal magmatic systems, we develop a new thermodynamic framework for modeling the distribution of C-H-O-S-N among the atmosphere, magma ocean, and metallic core of rocky planets during planet formation. This new framework integrates the thermodynamic data and state-of-the-art petrological models from the literature on volatile element behaviors in gases, silicate melts, and metallic liquids. Given that rocky planets are likely built from materials of variable compositions and redox conditions, it is expected that graphite, sulfide/sulfate, and Fe metal could reach saturation in the magma ocean under certain conditions. Upon saturation, these phases will be separated from the magma ocean, yielding a decrease of volatile budgets in the gas-melt system. We will show that this new framework incorporates the complexities as mentioned above and can simultaneously compute the atmosphere pressure, atmosphere composition, volatile compositions of the magma ocean and core, post-degassing oxygen fugacity, and mass fraction of the core. Preliminary results will be discussed to demonstrate C-H-O-S-N distribution in planetary magma oceans during accretionary growth.

[1] Sun, C. and Lee, C.T.A., 2022. Redox evolution of crystallizing magmas with C-H-O-S volatiles and its implications for atmospheric oxygenation. Geochimica et Cosmochimica Acta, 338, pp.302-321.