Silicate melt-vapour equilibrium: Simulations and equations of state

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Silicate fluids are of fundamental importance in modelling the formation of rocky planets and satellites. For such modelling, it is relevant to know whether the fluid exists in a liquid, vapour or supercritical state, as well as the fluid's bulk properties. When such information is required by planetary modelling codes, it is incorporated via an equation of state.

Ab initio molecular dynamics simulations suggest that the isochoric heat capacities of near-critical silicate liquids greatly exceed the Dulong-Petit limit [1, 2]. This observation violates the assumptions governing currently-available equations of state for such fluids, e.g. [3, 4]. If silicate liquid heat capacities are as large as the simulations indicate, it has substantial implications for the relationship between heat flow and temperature in models of planet and satellite formation.

We review the arguments in support of high liquid capacities. We then discuss a new equation of state for silicate fluids, in the system Mg−Fe−Si−O_2, that accounts for such heat capacities.

[1] Karki *et al*. (2007) *Phys Rev B* **76** 104205. [2] Green *et al*., submitted. [3] Melosh (2007) *Meteorit Planet Sci* **42** 2079-2098. [4] Connolly (2016) *J Geophys Res-Planet* **121** 1641-1666.