Developing an Integrated Thermochemical Code for Modeling Lunar Magma Ocean Evolution

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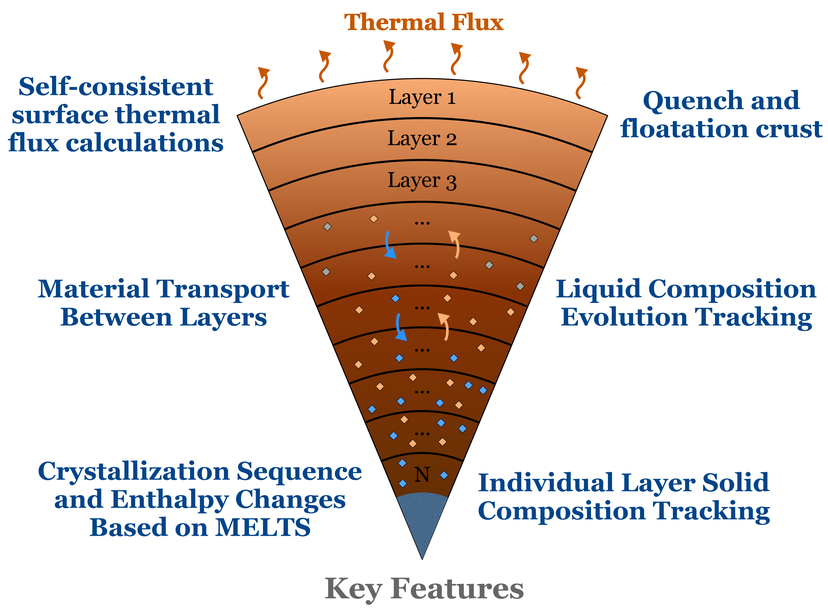
Summary (Abstract #2846)

We are developing a code that can both thermally and chemically evolve a Lunar Magma Ocean of an arbitrary starting composition, depth, and temperature. This open source code will be integrated with the MELTS geochemical model. Code outputs will include mineral assemblages over time and overall solidification time.

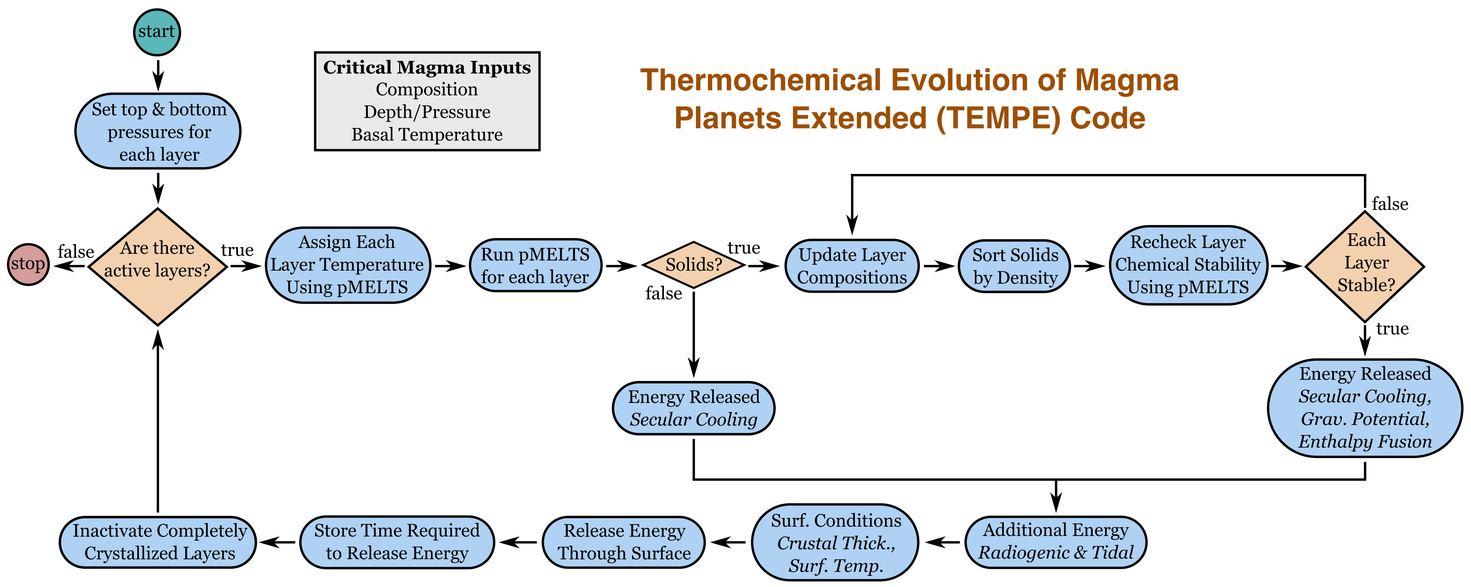
Why is this code needed?

For nearly 50 years the Lunar Magma Ocean (LMO) model has been developed by analyzing Apollo samples [e.g., **1**], conducting petrological experiments [e.g., **2**], and running computer models [e.g., **3**]. Yet, a fully-integrated thermochemical model, in which both crystallization of minerals and thermal flux calculations are done self-consistently is not currently available. Having such a model would be beneficial to better understand fundamental questions in lunar science (e.g., how long did the LMO last?) and help to characterize the early evolution of planets in general.



What is this code going to do?

For a given initial chemical composition, depth, and temperature of the LMO, this code will determine mineral assemblages as a function of depth and the corresponding thermal energy that is released. It will then calculate the overall solidification time. Phase relationships will be calculated using the MELTS thermodynamic models of silicate systems, which have been calibrated with a variety of thermodynamic and phase equilibrium constraints [**4**]. We use alphaMELTS (v2.0) [**5**] as an interface that calls pMELTS (v5.6.1) [**6**]. The code algorithm is shown below.



What was the initial composition of the LMO?

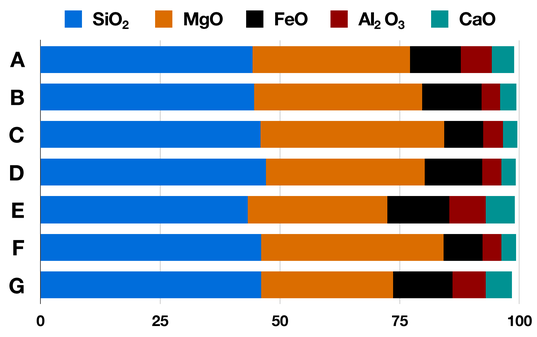


***Figure 1*: Seven different estimates of the initial LMO composition from the literature. Minor components (e.g., TiO_2 & Cr_2O_3) are used in MELTS modeling but are not shown. MnO was set to zero because adding it is not recommended for MELTS. Trace elements (e.g., Ni & Co) were not included.**

Sources

[**A**] Taylor Whole Moon (TWM) from Taylor, S. R. (1982) *Planetary Science: A Lunar Perspective*. as modified in Elardo, S. M. et al. (2011) *Geochim. Cosmochim. Acta*, 75(11), 3024–3045.
[**B**] O'Neill, H. St. C. (1991) *Geochim. Cosmochim. Acta*, 55(4), 1135–1157. as modified in Schwinger, S. & Breuer, D. (2018) *AGU Fall Meeting*, P31G-3778.
[**C**] Lunar Primitive Upper Mantle (LPUM) from Longhi, J. (2006) *Geochim. Cosmochim. Acta*, 70, 5919–5934. as modified in Elardo, S. M. et al. (2011) *Geochim. Cosmochim. Acta*, 75(11), 3024–3045.
[**D**] Elkins-Tanton, L. T., et al. (2011) *Earth Planet. Sci. Lett.*, 304(3–4), 326–336.
[**E**] Morgan, J. W., et al. (1978) *Moon Planet.* 18, 465–478.
[**F**] Ringwood, A. E. & Kesson, S. E. (1976) *Lun. Planet. Sci. Conf.*, 1697–1722.
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Outlook

TEMPE is being written in Python and will be made available as open source software. MELTS-family models are actively being updated and extended and as such their accuracy and range of applicability will improve with time. Thus, TEMPE will be a valuable tool for the planetary science community to study not only the thermochemical evolution of the Moon, but also the Earth and exoplanets.

How does chemistry affect LMO cooling?

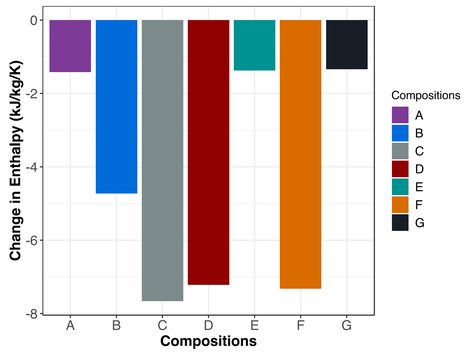

***Figure 2*: Change in enthalpy calculated in MELTS for a 100 gram mass of magma as it cools from 1700 to 1690 K at a pressure of 3 GPa for 7 different assumed initial compositions of the LMO. Oxygen fugacity of one log-unit below Iron-Wüstite (IW) buffer used for all calculations.**

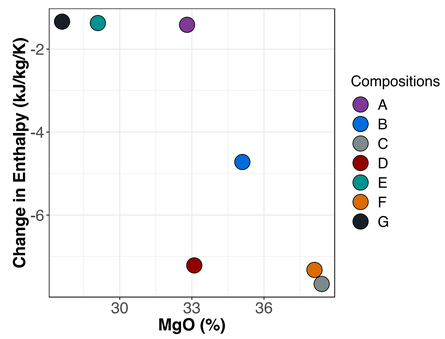

***Figure 3*: A primary driver of the differences in enthalpy released between the 7 compositions is the MgO content. Higher MgO values result in formation of orthopyroxene, while lower values do not.**

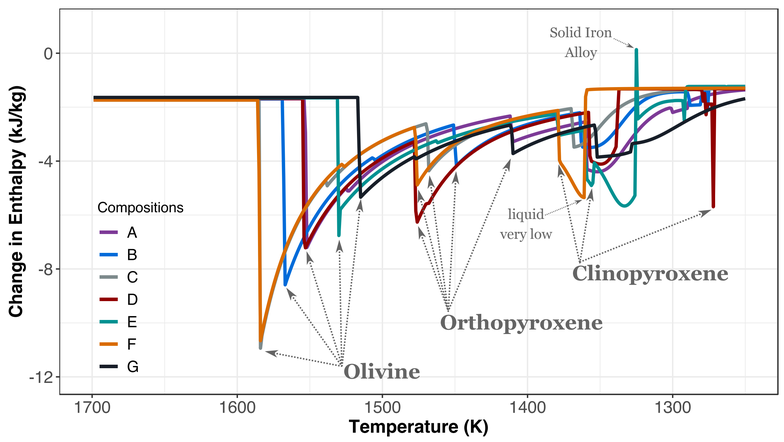

***Figure 4*: Thermal energy that is released vary for cooling magmas of different initial compositions. Shown here are MELTS cooling calculations for the 7 compositions at a fixed pressure of 1 GPa.**

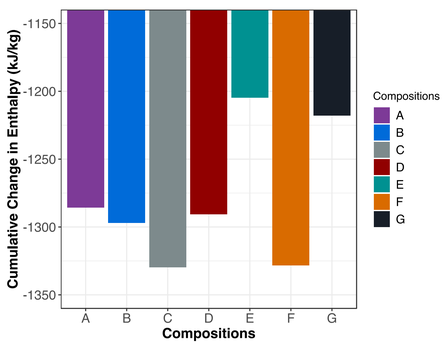

***Figure 5*: Variations in the released thermal energy for different compositions do not average out. Here we show that cumulative changes in energy differ based on the initial composition. Data from the MELTS calculations performed for magmas cooling from 1700 to 1250 K (see figure to the left).**

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References

[**1**] Wood J. A. et al. (1970) *Lun. Sci. Conf.*, 1, 965–988. [**2**] Lin, Y. et al. (2017) *Earth Planet. Sci. Lett.*, 471, 104–116. [**3**] Perera, V. et al. (2018) JGR-Planets, 123, 1168–1191. [**4**] Ghiorso, M. S. & Sack, R.O. (1995) Contributions Mineral. Petrol., 119(2–3), 197–212. [**5**] Smith, P. M. & Asimow, P. D. (2005) Geochem. Geophys. Geosyst., 6, Q02004. [**6**] Ghiorso, M. S. et al. (2002) Geochem. Geophys. Geosyst., 3(5), 1030.