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Partition Coefficients of Heat Producing Elements during Lunar Magma Ocean Crystallization and Their Influence on the Present-Day Selenotherm

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Introduction

The selenotherm is the temperature to depth relationship (thermal profile) in the lunar interior. Constraining the selenotherm is fundamental in understanding both surface and deep interior processes on the Moon. The selenotherm is a function of the radiogenic heat generated in different layers of the solid body of the Moon and their respective thermal properties. Our study aims to better constrain the selenotherm, which in turn would improve the current understanding of the following:

- Petrological processes occurring in the lunar mantle and associated igneous activities.
- Thermoelastic and chemical properties of the early moon and their evolution through time.
- Models of the lunar mantle dynamics and evolution in combination with surface heat flow measurements.

Uncertainties of the selenotherm which were independently estimated from inversions of seismic, gravity, and electromagnetic data span up to 800 °C; too large to apply petrologic models or geodynamic simulations. Factors affecting the nature of the present-day selenotherm are bulk concentration and distribution of heat producing elements (HPEs: U, Th, K), petrology of individual mantle stratigraphic horizons, thermal conductivity of the respective layers, and overturning of the high-density ilmenite-bearing cumulates (IBCs). The uncertainty of HPE distribution in the lunar mantle and crust poses a major roadblock for characterizing the lunar selenotherm.

We performed high pressure-temperature experiments to determine HPE partition coefficients for the minerals crystallizing from the lunar magma ocean at low oxygen fugacity conditions relevant for the lunar interior. Two different bulk silicate moon HPE concentrations are applied:

- **McDonough and Sun (1995) bulk silicate earth: U = 20.3 ppb, Th = 79.5 ppb, K = 25.26 ppm**
- **Faure et al., (2020) bulk silicate earth: U = 11.42 ppb, Th = 43.2 ppb, K = 14.21 ppm**

K concentrations were calculated as K/U = 1244.2 for lunar materials to account for its volatile nature (Korotev, 1998). The selenotherms were generated by incorporating the HPE estimates of different mantle stratigraphic layers into a 1D thermal conduction equation for a spherical shell model. To evaluate selenotherms for different overturn scenarios: we consider three models: no overturn, overturn of 50% of the IBCs, and complete overturn.

Methods

- Piston cylinder experiments conducted at The University of Arizona at 0.5 GPa in between 1200 - 1220°C.
- Graphite capsule were used, and experiments were equilibrated for 24 hours.
- Microprobe, Laser-ICP-MS, and SIMS techniques were used to characterize major, minor, and trace elements.
- Partition coefficients between glass, clinopyroxene, and plagioclase were determined for U, Th and K.
- Minimum and maximum partition coefficients reported in the literature were used for olivine, orthopyroxene, and quartz.

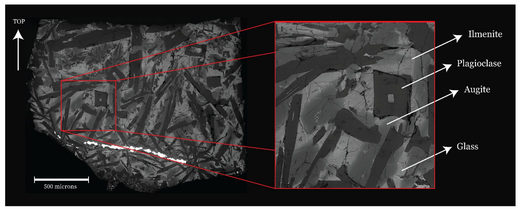

Figure 1. Back-scattered electron image of LMO experiment showing phases plagioclase, pyroxene, ilmenite and glass at 1220°C and 0.5 GPa, run for 24 hours used to determine HPE partition coefficients

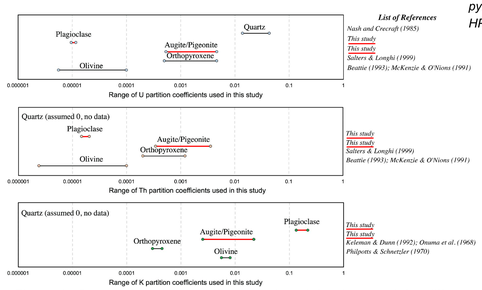

Figure 2. Range of partition coefficients selected for the model for different minerals crystallizing from the LMO

The conductive temperature is calculated systematically along a depth profile as:

$$T_{i+1} = T_i + (H_i * \rho_i * \Delta r^2) * (6.0\ k_i)^{-1}$$

where T=temperature [K], H=heat production [W kg^{-1}], ρ=density [kg m^{-3}], k=thermal conductivity [W m^{-1} K^{-1}], and i is the depth increment.

The process starts with an initial guess and iterates as:

1. Initial linearly increasing temperature and pressure from surface to core
2. Calculate density profile of the composite minerals via an equation of state
3. Recalculate thermal and pressure profiles
4. Repeat 2-3 until convergence

The resultant temperature profile represents a present-day snapshot of lunar conditions. The profiles will later be used as input to determine time-dependent thermal evolution via geodynamic modeling using ASPECT.

Results

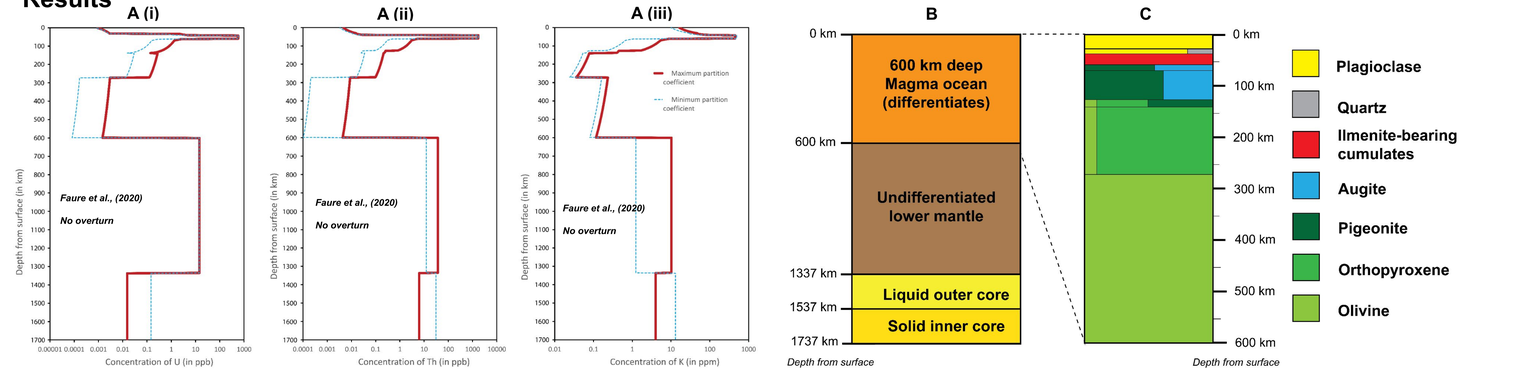

Figure 3. [A] Distribution of HPEs (U, Th, and K) within the lunar interior for maximum and minimum partition coefficients models. [B] Modeling was performed using a 600 km-deep magma ocean crystallization model (Charlier et al., 2018) and LPUM bulk composition. Assumptions include an undifferentiated lower mantle below the 600 km LMO and a 400 km radius of metallic core. Lunar bulk silicate HPEs concentrations are taken from Faure et al., (2020). [C] Modal mineralogical abundance of 600 km LMO from Charlier et al., (2018) study.

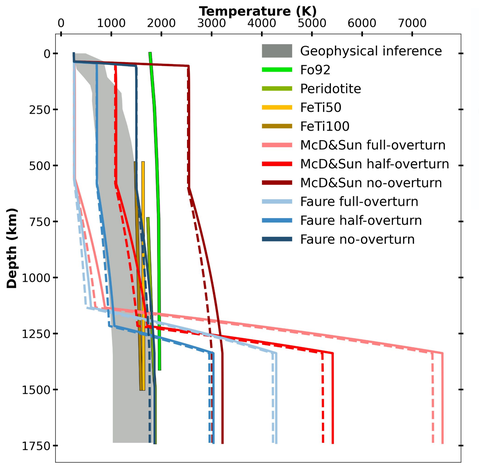

Figure 5. Selenotherms for McDonough and Sun (1995) in red and Faure et al., (2020) in blue. Dashed lines indicate models from minimum partition coefficients and solid lines for models from maximum partition coefficients. Solidus curves for lunar mantle minerals - Fo92: forsterite, FeTi: ilmenite-rich cumulate, peridotite - are also shown.

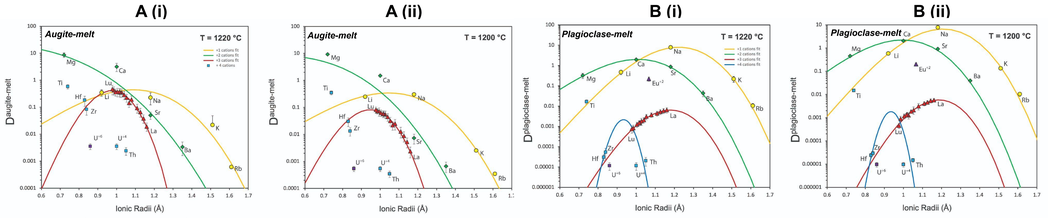

Figure 4. Onuma diagrams for augite-melt and plagioclase-melt. Lattice site parameters from parabola curve fitting for plagioclase and augite are listed in the table below:

	Plagioclase			Augite			
	D^0	E	r^0	D^0	E	r^0	T(°C)
+1 cations	7.971	102	1.22	0.44	53	1.088	1220
	6.599	94	1.21	0.34	53	1.045	1200
+2 cations	2.014	91	1.01	23.29	24	0.205	1220
	2.231	88	1.00	8.50	37	0.424	1200
+3 cations	0.006	171	1.18	0.42	271	0.975	1220
	0.006	168	1.19	0.08	235	0.947	1200
+4 cations	0.002	1490	0.93				1220
	0.002	1555	0.93				1200

References

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Conclusions

- The selenotherm is strongly influenced by the overall bulk Moon HPE abundance, which in turn controls the HPE concentration within the IBC layer. Abundance determined from McDonough and Sun (1995) BSE concentrations generate very hot selenotherms, in contrast to the relatively colder selenotherms using Faure *et al.,* (2020) concentrations.
- Selenotherms using Faure's U and Th concentrations support the idea of EL rather than carbonaceous chondrites being the dominant building block of Earth (Dauphas, 2017).
- The no overturn and 50% overturn scenario with Faure's HPE abundance produces the most reasonable selenotherms, closely following the upper and lower boundaries of geophysical inference (grey).

Future Work

- Experimental measurements of the partition coefficients applicable for the late crystallizing minerals quartz and ilmenite may narrow down the uncertainty in the selenotherm.
- Additional selenotherm scenarios need to be explored where the overturning IBCs become intermixed within the upper and lower mantle mineralogies.