

ASSESSING CRYSTALLIZATION MODELLING SOFTWARE'S ACCURACY FOR THE DETERMINATION OF MULTIPLE SATURATION POINTS IN LUNAR AND MARTIAN BASALTS. D.

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Introduction

The physical conditions at which multiple saturation points (MSPs) occur on the liquidus of primary magmas are useful as an empirical approximation to the conditions at which the partial melting of their source rocks occurred [1]. These conditions can be obtained through crystallization experiments on the compositions of basalts that have not undergone fractional crystallization or any sort of alteration since their partial melt origin.

On Earth, basalts with these characteristics are very uncommon, but it is believed that some have been found on mid-ocean ridges, which have allowed for some experimentation into their melting conditions [2]. In the case of the Moon, many mare basalts and picritic glasses are believed to be the products of deep mantle melting and many pristine samples are believed to be products of near-primary melts (e.g. [3]). Therefore, their MSPs conditions have been used to constrain the conditions of mantle melting. For Mars, a rover-measured composition for the Gusev basalts [4] and some martian meteorite compositions, which have been corrected for fractional crystallization effects, were used for the study of their near-primary compositions [5].

Using crystallization modelling algorithms

To study the conditions where a near-primary melt was formed when the composition of the source region is not known, it is necessary to take an inverse approach by crystallizing the melt at different temperature/pressure conditions until an MSP is reached on its liquidus. The phases present there should be the ones that were in equilibrium in the mantle with the partial melt during its formation, assuming the residual source region contained two or more mineral phases. Approaching this through high P-T experiments is the typical inverse method approach and can reveal the P-T conditions of liquidus multiple saturation within a few 10's of degrees and a 0.1 – 0.2 GPa. However, crystallization modelling software has been available for a few decades and can be used to approach similar results more easily with far less cost than experiments, provided the calibrations for each software are appropriate to the compositions and conditions of crystallization.

pMELTS [6, 7] is a variant of the MELTS family of algorithms based on a dataset of over 2500 experiments, and is focused on modelling melting and crystallization of terrestrial mantle spinel peridotites, although there are lunar basalt experiments within its calibration

dataset. The accuracy of this algorithm in reproducing MSP conditions has been previously explored for MORB compositions [2] and for martian basalts [5], but not yet for lunar basalts.

The MAGPOX program and its algorithms were developed for modelling crystallization of olivine-saturated melts based on the equations in Longhi [8–10]. It is used for modelling equilibrium crystallization of basaltic melts and has been shown to successfully reproduce the crystallization sequence of lunar melt compositions. Asimow and Longhi [2] have previously explored the accuracy of MAGPOX in reproducing MSP conditions for MORB compositions and its consistency with pMELTS results, but this has not been done yet for lunar or martian basalt compositions. In this work, we explore the results of both pMELTS and MAGPOX modelling on a set of lunar and martian basalt compositions and determine how accurately they reproduce their experimentally-determined MSP conditions.

Methods

A set of 20 lunar basalt compositions and 4 martian basalt compositions with known experimental results for MSP conditions were analyzed through both software. In order to automate the process, the Fortran version of MAGPOX was edited to bypass input requests and a Python script was written to sequentially process each composition through the pressure range of 0.2 GPa to 3 GPa with a 0.2 GPa step resolution and temperatures between 1700 °C and 1000 °C with a 10°C step resolution. For pMELTS, we used the “MELTS-batch” build of the algorithm (from the MELTS repository), edited it to default calculations to the pMELTS version, and wrote a similar Python script to run it sequentially through the same conditions as for MAGPOX, except for the temperature lower limit, which was set to 1200 °C. Results were then used to build phase diagrams where the MSP conditions were determined.

Results

All compositions produce MSPs during modelling. However, only a few of compositions produce matches to the MSP conditions of their experiments in both algorithms, and all of the good matches occur in the lower end of the lunar and martian MSP pressure range. Even though there are experimental MSPs at pressures up to 2.5 GPa, pMELTS does not produce MSP conditions at pressures higher than 1.3 GPa. Similarly, many MAGPOX results occur at 1.6 GPa, but do not

exceed that value. Most MSPs occur between olivine and clinopyroxene in pMELTS and between olivine and pigeonite in MAGPOX, although pMELTS describes pigeonite as ‘clinopyroxene’. Phases are consistent with those in the corresponding experimental studies. As was noted by Balta and McSween [5], pMELTS calculates chromite saturation much too early at very high temperatures in almost all compositions, and is not considered as a liquidus phase because it is only present in a few experiments.

The temperature differences between experiments and calculations increase with the temperature of experimental MSPs (Figure 1), with pMELTS temperatures lower than MAGPOX at the higher temperatures.

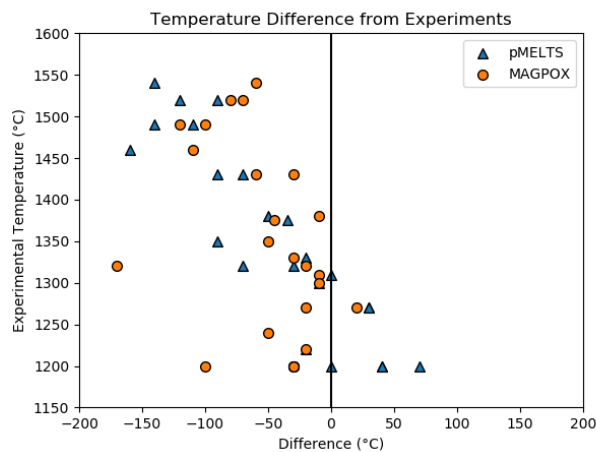


Figure 1: Temperature difference of MSPs calculated through pMELTS and MAGPOX with the experiments.

Discussion

All MSPs involve olivine and pyroxene, and it is mostly MgO and CaO concentrations that control the saturation curves of both minerals. This is likely the reason the MgO/CaO ratio shows the best correlation for temperature conditions. Since no other minerals are relevant in the liquidus of the melt in the experiments, besides occasionally spinel/chromite, there is no clear correlation between other elements and the MSPs. Figure 2 shows that both programs calculate lower temperatures for the higher ratios, also leading to lower pressure estimates.

In the case of pMELTS, we compare the natural compositions used in the experiments to the calibration database to assess if the differences in MSP conditions can be explained through compositional differences. We find that the compositions are in fact encompassed within the database, however, the experimental results conditions are not. Using the MgO/CaO ratio to compare lunar and martian basalt compositions to

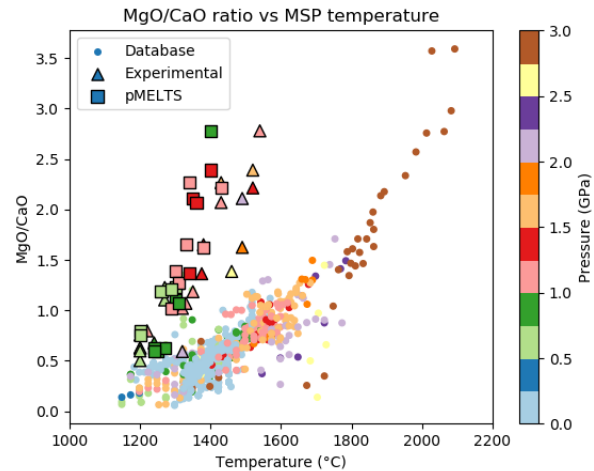


Figure 2: Comparison of experimental composition and results, with a subset of the pMELTS experimental database that contain olivine and clinopyroxene.

database experiments that contained both olivine and clinopyroxene (Figure 2), we see that temperature increase of the experimental MSPs lies off of the general trend of the pMELTS dataset, but the calculations tend to shift the results in the opposite direction. Nonetheless, temperature results approach the experimental trend rather than the database one and the differences are likely to be related to the database focus on lherzolite melting instead of harzburgite or pyroxenite, which would be more appropriate for lunar and martian mantles.

A similar analysis for the MAGPOX differences is currently underway. It seems that both software can be fairly accurate for lunar and martian basalts formed on shallow conditions but underestimate the conditions for deeper forming melts.

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