AN EVALUATION OF THE IGNEOUS CRYSTALLIZATION PROGRAMS -- MELTS, MAGPOX, AND COMAGMAT PART I: DOES ONE SIZE FIT ALL?

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Introduction: Computer models are commonly used in the geologic community to simulate magma crystallization. The computer programs/models evaluated in this study are from 3 sources: MELTS [1], MAGPOX [2], and COMAGMAT [3]. Multiple versions exist of the models, and versions available from the authors differ from those available on the internet. It is not always clear which version of a model is used in different studies, or if the model was adapted to fit a certain composition. Likewise, it is unknown if a different model or version should be used depending on the melt composition or its crystallization conditions (P, fO_2). Here we compare and evaluate the 3 computer models designed to simulate equilibrium crystallization of basaltic magmas. The bottom line to this study was to determine whether it is appropriate to apply one model to a range of bulk compositions and oxidation states. *It is not!* Each model has it strengths and weaknesses and should not be used indiscriminantly.

This Study: The crystallization programs evaluated in this study are MELTS (Mac version 5.1) [1], MAGPOX (disk version .1102) [2], and COMAGMAT (internet version 3.3) [3]. Each program was originally developed with a different approach to modeling mineral-melt interaction. ***MELTS*** relies heavily on thermodynamic modeling and experimental data collected on anhydrous "basalt-like" compositions [1]. This model was developed for terrestrial magma compositions ranging from potash ankarites to rhyolites, at pressures up to 40 kbar with an error of ± 10ºC for liquidus temperatures [1]. The basis for ***MAGPOX*** is the projection of parameterized, experimentally determined liquidus boundaries in the system CaO-MgO-Al_2O_3-SiO_2 [2]. MAGPOX was developed primarily for simple lunar basaltic systems, with an error of ± 13ºC for liquidus temperatures, and with olivine as the first crystallizing phase [2,3]. ***COMAGMAT*** is based on a combination of experimentally determined, mineral-melt geothermometers used to calculate equilibrium temperatures and phase relations. It is intended for terrestrial melt compositions ranging from primitive basalts to dacites, at pressures up to 12 kbar and an error of ± 10ºC for liquidus temperatures [4].

Methodology: Three rock (i.e., parent melt) compositions were chosen with contrasting compositions and fO_2 conditions of formation: 1) martian meteorite Nakhla [5]; 2) angrite LEW 86010 [6]; and 3) Apollo 15 basalt 15555 [7]. These 3 rocks were modeled at 3 values of fO_2: QFM, QFM-2, and IW. This makes for *a 3x3x3 matrix of models x comps. x fO_2*. Due to the extent of this study, the accompanying abstract by Slater et al. [this volume] addresses the fO_2 portion of these evaluations. In addition, equilibrium crystallization was simulated at a pressure of 1 bar and the following estimated values for magmatic fO_2: QFM for Nakhla [8], IW+1 for LEW 86010 [9], and IW for 15555.

The precision to which these modeling programs predicted the crystallization sequences, modal abundances, and compositional ranges of minerals in each sample was assessed. Modeled mineral abundances and compositions were compared to those observed in each sample, and modeled crystallization sequences were compared with those obtained from crystallization experiments.

Results: Modeled crystallization sequences and 'modeled versus observed' modal abundances and compositions of major minerals are shown in Figure 1 and Table 1, respectively.

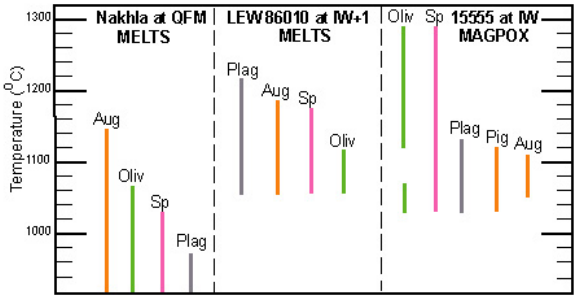

Figure 1. Best-modeled crystallization histories for major minerals (>5%) in Nakhla, LEW 86010, and Apollo 15 basalt 15555 at estimated magmatic oxygen fugacities.

MELTS produced the closest match to the crystallization sequence observed phase assemblage and compositions for ***Nakhla***. The average modeled clinopyroxene and olivine compositions fall within the observed range of compositions [10,11]. Although MAGPOX and COMAGMAT modeled reasonable clinopyroxene compositions, they did not crystallize olivine. Orthopyroxene compositions from MELTS are more Fe-rich than the range of measured compositions, but neither MAGPOX nor COMAGMAT predicted

any orthopyroxene. Olivine compositions predicted by MELTS fall within observed ranges. Plagioclase compositions from MELTS overlap observed compositions in Nakhla and extend to more Ca-rich compositions. Plagioclase compositions predicted by MAGPOX and COMAGMAT are too albitic and do not overlap observed compositions.

MELTS was the only program that predicted the correct crystallization sequence for ***LEW 86010*** and compares well with observed and experimental mineral compositions. MAGPOX predicted LEW 86010 to be nearly multisaturated, and COMAGMAT crystallized augite with only a fraction of late-stage plagioclase. MELTS predicted comparable plagioclase abundances, and MELTS and MAGPOX predicted correct compositions. MELTS crystallized pyroxene near the observed abundance, but none of the models predicted observed pyroxene compositions: they are similar, however, to experimental results. Olivine was best modeled by MELTS. MAGPOX crystallized less than half the observed amount of olivine with higher Fo contents and COMAGMAT did not crystallize any. Finally, both MELTS and MAGPOX crystallized too much spinel.

MAGPOX appears to reproduce most closely the crystallization sequence and compositional and modal data reported for ***Apollo 15 basalt 15555*** [12,13,14]. MAGPOX and COMAGMAT predicted the correct crystallization sequence, but COMAGMAT crystallized no spinel. Olivine and spinel crystallized nearly simultaneously as did pyroxene and plagioclase using MAGPOX. MELTS did not predict the crystallization sequence and crystallized whitlockite but not ilmenite. Plagioclase is slightly more calcic than observed compositions using MAGPOX, but olivine and pyroxene fall within observed compositional ranges. MELTS and COMAGMAT produced clinopyroxene that is too calcic. Although both MELTS and MAGPOX predicted modal proportions similar to what is seen in 15555 [15,16], MAGPOX produced slightly higher amounts of olivine and slightly lower amounts of pyroxene.

Conclusions and Work in Progress: Although this study is a first-order evaluation of the 3 crystallization models commonly used by petrologists, it is readily apparent that "one size does NOT fit all." – i.e., no single model is applicable to all rocks. Additionally, the study reported by Slater et al. [this volume] reinforces this conclusion and permits an extension of the above evaluation into the realm of fO_2 variation. It is clear that one model should not be used for all melt compositions and fO_2 conditions. Our study has demonstrated that additional evaluations are necessary before we can use these programs with confidence for particular compositions or fO_2 conditions and caution in use of these programs is definitely warranted.

References: [1] Ghiorso & Sack (1995) *CMP;* [2] Longhi (1991) *Amer. Min;* [3] Longhi (1988) *GCA* + included refs; [4] Ariskin et al. (1993) *Comput. Geosci.;* [5] Stockstill (2003) *MAPS;* [6] McKay et al. (1988) *LPSC XIX;* [7] Janghorbani et al. (1973) *GCA;* [8] Reid & Bunch (1975) *Meteor.;* [9] McKay et al. (1994) *GCA;* [10] McSween & Treiman (1998) *Martian Meteor.;* [11] Sautter et al. (2002) *EPSL;* [12] Chappell et al. (1972) *Sci.;* [13] Longhi et al. (1972) *A-15 Lunar Samples;* [14] Ryder (1985) NASA JSC Pub. 72; [15] Heuer et al. (1972) *A-15 Lunar Samples;*.[16] Nord et al. (1973) *PLS Conf. 4th*.

Table 1. Observed and modeled mineral abundances (vol. norm. to 100%) and compositions for major minerals present in each sample. Best fit results are bold red.

	Observed	MELTS	MAGPOX	COMAGMAT
Nakhla	**QFM**	**QFM**	**QFM**	**QFM**
pyroxene	69-79% $Wo_{4-40}En_{38-15}$	50% $Wo_{38-43}En_{39}$	**57.2% $Wo_{38-39}En_{36-20}$**	50% $Wo_{26-43}En_{37-35}$
olivine	10-16% Fo_{41-14}	**10% Fo_{34-16}**	21.1% Fo_{54-18}	0%
plagioclase	4% An_{28-15}	**28% An_{47-15}**	20.3% An_{12-8}	20% An_{8-5}
LEW 86010	**QFM-3**	**QFM-3**	**QFM-3**	**QFM-3**
plagioclase	21-26% An_{100}	**21% An_{100}**	55% An_{100}	0.1% An_{100}
augite	45-58% $Wo_{31-42}En_{35-20}$	61% $Wo_{30-60}En_{5-5}$	**30% $Wo_{50-52}En_{39-28}$**	99.9% $Wo_{40-49}En_{36-28}$
olivine	20-22% Fo_{31}	**15% Fo_{40-25}**	5% Fo_{62-40}	29% Fo_{50-22}
Apollo 15 15555	**IW**	**IW**	**IW**	**IW**
olivine	12-20% Fo_{71-59}	8.2% Fo_{74-45}	26.3% Fo_{74-47}	**12.4% Fo_{74-52}**
plagioclase	26-35% An_{94-78}	23.5% An_{87-86}	**35.5% An_{96-90}**	20.3% An_{88-83}
pigeonite	40-55% $Wo_{10-36}En_{51-30}$	46.1% $Wo_{7-13}En_{64-46}$	**22.2% $Wo_{9-15}En_{58-44}$**	0%
augite		17.4% $Wo_{36-40}En_{42-37}$	**13.4% $Wo_{36-37}En_{43-37}$**	65.1% $Wo_{19-39}En_{39-38}$