LET'S SPICE THINGS UP: SIMULATING PLANETARY IGNEOUS CRYSTALLIZATION ENVIRONMENTS. J. D. Davenport[1,2,3], J. Longhi[4], C. R. Neal[2,3], D. Bolster[2] and B. L. Joliff[5] [1]Centre de Recherches Petrographiques et Geochimiques, 54500 Vandoeuvre-les-Nancy, France, [2]Dept. of Civil and Environmental Engineering & Geological Sciences, University of Notre Dame, Notre Dame, IN 46556, USA, [3]NASA Lunar Science Institute, U.S.A., [4]Lamont-Doherty Earth Observatory, Palisades, NY 10964, USA, [5]Dept. of Earth and Planetary Sciences, Washington University, St Louis, Missouri 63130, USA (jessedvnprt@gmail.com; neal.1@nd.edu).

Introduction: The MAGFOX [1], MAGPOX [2], BATCH [3], and FXMOTR [4] modeling codes were first developed in the early 1990s by experimental and lunar petrologist John Longhi to examine magma as it evolved via fractional and/or equilibrium crystallization. The programs were originally written using the cumbersome FORTRAN 77 programming language, but here they have been translated into the user friendly MATLAB programming environment.

The legacy of these programs is important: the FORTRAN versions of MAGFOX and MAGPOX, combined with geochemical and petrographic techniques, have been used repeatedly in the past to study lunar igneous suites and their implications for the evolution of the Moon (e.g., magma ocean crystallization, the petrogenesis of the lunar highlands, and mare basalt source regions). The programs have also been used to study igneous suites on the Earth and other terrestrial planetary bodies where olivine is initially on the liquidus.

The purpose and goals of this translation can be summarized in three points: 1) To break free from the cumbersome and outdated FORTRAN 77 programming language, 2) to bring these programs to a broader scientific audience by using a much more accessible programming language such as MATLAB and 3) provide access to these programs to users who have little to no programming experience via graphical user interfaces (GUIs). This new, user-friendly code, when combined with geochemical analyses, will be able to provide the phase relationships needed to better understand the petrogenesis of many igneous suites.

Copies of these programs are available from the authors and on the Lunar and Planetary Institute (LPI) website within the "Computational Tools" as a graphical user interface and windows executable file (http://www.lpi.usra.edu/lunar/tools/crystallizationcalculation). The programs are written in MATLAB, but the basic code can also be executed in the open source Octave programming language (located here: https://www.gnu.org/software/octave/).

The Programs: [5] and [6] give detailed information on the applicability of different programs on various magmas. SPICEs provides a GUI that users with no programming experience can harness to model crystallization processes ([7]; Fig. 1). MAGFOX uses Rayleigh fractional crystallization, while MAGPOX uses equilibrium crystallization in 1% crystallization steps — to calculate the major element oxide evolution of the liquid and mineralogy in several projections (e.g., the Ol-Pl-Wo-Sil system; e.g. Fig. 2). The programs can be used to derive crystallization sequences for different magmas (Fig. 3).

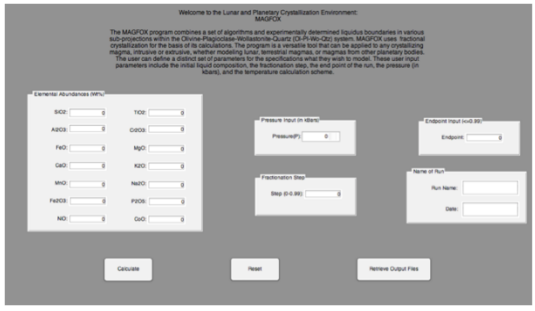


Figure 1: An image of the MAGFOX graphical user interface layout.

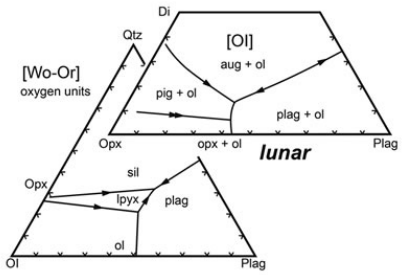


Figure 2: An example of the Ol-Pl-Wo-Sil system, from which the user can derive a crystallization sequence for a given magma.

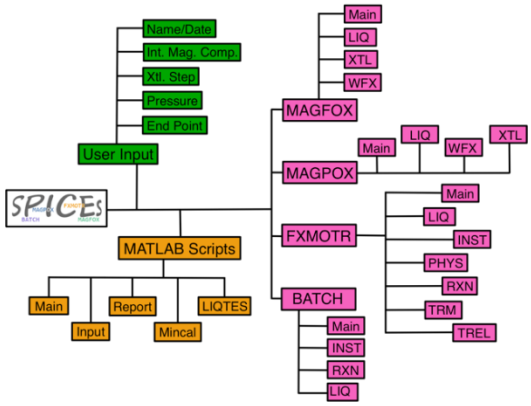
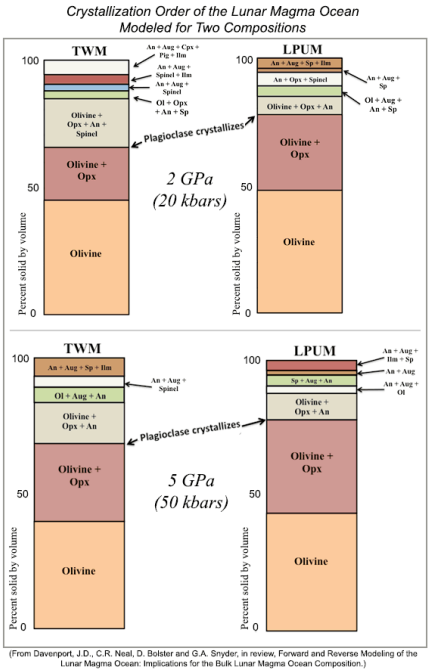


Figure 3: A schematic/flow chart describing the methods, process, and files of the SPICEs programs.

FXMOTR uses a combination of equilibrium and fractional crystallization in 1% crystallization steps to calculate the evolution of major and trace elements of a liquid and crystallizing mineralogy.

BATCH is a high pressure version of MAGPOX. Consult [7] for more details on the organization of the code. Appendix A of [7] and references therein contain descriptions of all equations used in each program. [7] also details the construction of the GUIs (Fig. 2) for each program.

FXMOTR and the LMO, A case study: The Lunar Magma Ocean (LMO) has posed an interesting study ever since the return of anorthositic samples and the subsequent development of LMO theory. Despite several decades of LMO research, there are still a number of unsolved questions. For example, [8] sets the LMO depth at 400 km, while [9] sets the depth at 1000 km. This, coupled with variations in the initial LMO composition, produce variations in the mineralization sequences for LMO crystallization. Here, FXMOTR is used to calculate various mineralization sequences to crystalize the LMO assuming LMO depths of 400 km and 1000 km (20 and 50 kbar, respectively) and the TWM and LPUM LMO bulk initial compositions from the literature. Fig. 4 (below) highlights some of these results.



With the help of FXMOTR, it is found that an enrichment in alumina in the initial bulk LMO composistion produces plagioclase on the liqudus much earlier than a less Al-enriched composition. Similar effects can be seen with increased LMO depth. Furthermore, with an increased Al and depth, garnet becomes present in small quantites (usually 1-5 wt.%; more to come in the future on this aspect).

Recent GRAIL data are consistent with a bulk Moon Al_2O_3 composition of ~4 wt.% with an average crustal thickness between 34-43 km [10]. However, this assumes that the majority of Al_2O_3 is sequestered in the lunar crust and does not indicate the presence of an aluminous phase, i.e. garnet or spinel, in the lunar mantle. If garnet is present at depth, the bulk Al_2O_3 of the Moon must be increased. A higher Al_2O_3 content in the bulk Moon would facilitate earlier crystallization of plagioclase and other aluminous phases if the LMO was deeper than ~500 km. In turn, this would allow plagioclase to crystallize earlier and form the lunar crust eariler, thus yielding the inherent negative Eu anomaly in the mare source regions (requiring either a somewhat muted overturn of the cumulate pile or no overturn). Earlier crust formation would generate an insulating lid and promote a longer-lived LMO, as postulated by [11] and [9]. More recently [12], using MELTS, has proposed that the Moon is more enriched in FeO and Al_2O_3 than previously thought, consist with the results here. They argue that bulk Moon FeO can be constrained to 1.3-1.8 xBSE (Bulk Silicate Earth) and Al_2O_3 between 1 and 1.5 xBSE.

Summary & Conclusion: SPICEs has been an integral part in understanding the evolution of countless terrestrial, lunar, and other planetary magma compositions. The SPICEs source code has been converted from the now outdated FORTRAN 77 language into the user-friendly MATLAB programming environment. The SPICEs code allows the user to quickly calculate crystallizing phases of a magma based on its initial composition, pressure (depth), crystallization step, and model terminus. The examples presented within show that the SPICEs code is a valid tool for understanding the evolution of a number of varied magmas on a variety of planetary bodies.

Future Work: One of the key aspects future studies should address is updating the partition coefficients for the major and trace element modeling, which will be a big, albeit very important job. It will have to use the compositions of the crystallizing phases to calculate the correct partition coefficients using research from the University of Notre Dame for plagioclase [13] and Brown University for pyroxene [14], among others. Other technique updates, appropriate for SPICEs, will also be incorporated into the models.

References: [1] Longhi, J. (1991) *Am. Mineral., 76, 785–800* [2] Longhi, J. (1992) *PLPSC 22,* 343-353 [3] Longhi, J. (2002) *G^3*, 1-33 [4] Longhi, J. (2006) *GCA 70,* 5919-5934 [5] Slater et al. (2003) 34th LPSC, Abstract #1896 [6] Thompson et al. (2003) 34th LPSC, Abstract #1881 [7] Davenport et al. in prep. for *Comp. Geosci.* [8] Snyder G.A. et al. (1992) *GCA 56*, 3809-3823 [9] Elkins-Tanton L.T. et al. (2011) *EPSL 304*, 326-336 [10] Wieczorek et al., (2013) *Science 339*, 671-675 [11] Borg et al. (2011) *Nature 477*, 70-73 [12] Sakai et al. (2014) *Icarus 229*, 45-56. [13] Hui et al. (2011) *GCA 75,* 6439-6460 [14] Sun and Liang (2013) *GCA 119,* 340-358.