SIMULATING PLANETARY IGNEOUS CRYSTALLIZATION ENVIRONMENTS (SPICES): A SUITE OF IGNEOUS CRYSTALLIZATION PROGRAMS J. Davenport[1,2,3], J. Longhi[4], C. R. Neal[2,3], Bradley Joliff[5] and Diogo Bolster[2], [1]Centre de Recherches Petrographiques et Geochimiques, Nancy, France 54000; [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], FXMOTR [3] and BATCH [4] programs (further referred to as SPICEs) combine a set of algorithms and experimentally determined liquidus boundaries in various sub-projections within the Olivine-Plagioclase-Wollastonite-Silica (Ol-Pl-Wo-Sil) system. SPICEs use three general configurations for the basis of calculations: equilibrium crystallization for MAGPOX and BATCH, fractional crystallization for MAGFOX and a combination of fractional and equilibrium crystallization for FXMOTR. BATCH is a high-pressure version (>15 kBars) of MAGPOX. MAGPOX, MAGFOX and BATCH model major element evolution, whereas FXMOTR models a combination of major and trace elements. The programs are versatile tools that can be applied to any magma composition on the Moon, Earth or a variety of other planetary bodies. The user can define a distinct set of parameters for the scenario that they wish to model. These user input parameters include the initial liquid composition, the fractionation step, the model terminus and the pressure (in kbars).

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/). The programs are written in MATLAB, but the basic code can also be executed in the open source Octave programming language.

Aim of the Programs: There are a multitude of publications that have already used the SPICEs source code in application to terrestrial, lunar, and other planetary body magma evolution. In recent years, the syntax of programming languages such as FORTRAN 77 has become outdated and superseded by less cumbersome programming environments. The work presented here takes the SPICEs source code and converts it into the much more user-friendly MATLAB interface. The underlying goal in this conversion is to be able to promote the SPICEs code to a much larger and broader scientific audience. There are a number of programs available to model petrogenesis. All of these programs have their specific advantages and disadvantages, but it is up to the user to be aware of the strengths and weaknesses of each and plan which to use according to their modeling needs. [5] and [6] tried to answer this question by conducting an evaluation of a number of computer models on lunar and meteorite samples. They conclude that MAFOX and MAGPOX most readily recreate the observed values of major mineral abundances in lunar suites (e.g. Table 1). The combination of geochemical data with a user-friendly code can be a powerful tool to model the evolution of the magma in question, and thus provide a better understanding of the evolution of a crystallizing magma.

Organization of the Code: The code is composed of a series of MATLAB scripts and functions, which take as input data the bulk composition of the initial magma, the fractionation step, the model terminus and initial pressure (i.e., depth). Each source code is split into five scripts: 1) The Main code, 2) the LIQTES script, 3) the MINCAL script, 4) the REPORT script, and 5) the input script. The main SPICEs code calls all of the subsidiary scripts and initiates user input, parameter loading and model calculations. The output of MAGFOX and MAGPOX contains four files that are written to tab-delimited text files. FXMOTR and BATCH output includes seven tab-delimited text files. 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 Graphical User Interfaces (GUIs; Fig 1) for each program.

A MAGFOX Example: [8] first attempted to categorize Apollo 17 high-Ti basalts into Type A, B, and C on the basis of whole-rock geochemistry. Type A basalts were found to contain 50-60% increased abundances of incompatible trace elements compared to Type B basalts, although both possess similar major elemental concentrations [9]. [10] further divided the Type B group into Type B1 and B2, negating the need for models with varying degrees of partial melting and KREEP assimilation to

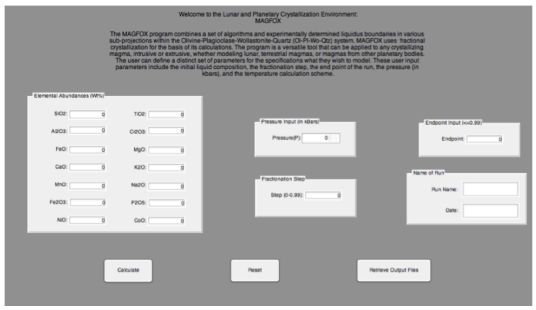

Figure 1. An image of the MAGFOX graphical user interface layout.

explain the range in the La/Sm ratio of Type B basalts. Type C basalts, of which only 5 are documented, were only found at Apollo 17 Station 4 (Shorty Crater) and contain elevated MgO and Cr_2O_3 relative to Type A and B basalts. [10] proposed a simple petrogenetic model of closed-system fractional crystallization to account for the compositions of Apollo 17 basalts. [10], unfortunately, only modeled the evolution of trace elements in Apollo 17 high-Ti basalts. More recently, [11] took a more in-depth look at fractional crystallization process in Apollo 17 high-Ti basalts, but have again only modeled trace elements. Using whole-rock geochemistry to define parental compositions for each group of Apollo 17 high-Ti basalt we model major elements via fractional crystallization using MAGFOX (Figure 2) and compare the crystallization sequences to crystallization sequence results for the trace element modeling.

The results of the MAGFOX modeling (Figure 2), [8] and [9] produce the same crystallization sequences within within 10% of each other. All three have olivine, armalcolite and spinel on the liquidus within the first 0-40% crystallization. Ilmenite, clinopyroxene, pigeonite and plagioclase replace spinel, olivine, and armalcolite in varying proportions after 40% crystallized until >90% crystallized. [10] did not record the presence of plagioclase on the liquidus, whereas the results presented here (and the models of [11]) produce a significant amount (>40%) at and after 50% crystallized.

The advantage to MAGFOX over trace element models is that trace element models rely on expensive geochemical analyses whereas MAGFOX only requires knowledge of a starting composition and pressure. However, the trace element modeling and MAGFOX provide an excellent comparison from which MAGFOX results can be used to better define the crystallization assemblage used in trace element modeling.

Summary & Conclusion: The SPICEs crystallization program have been an integral part in understanding the evolution of countless terrestrial, lunar, and other planetary magma compositions. We have converted the SPICEs source code from the now outdated FORTRAN 77 language into the user-friendly MATLAB programming environment. The SPICEs code allow the user to quickly calculate the 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.

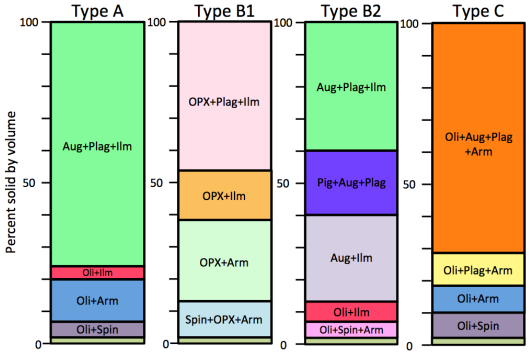

Fig 2. Apollo 17 Type A, B1, B2, and C crystallization sequences. Oli=olivine; Opx = orthopyroxene; Ilm =ilmenite; Pig = pigeonite; Sp = spinel; Arm = armalcolite; Plag= plagioclase; Aug = augite.

Future Work: As with all complicated modeling programs there will always be a number of bugs and issues with the code that cannot be foreseen or dealt with by the initial scientist/programmer working on the project. Therefore, future work includes releasing updated codes via publications and the web to the scientific community to find bugs/errors in the code. A future goal of this project is to keep SPICEs code updated with the latest published techniques.

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