**Transcript of MCS v.2019 FC Run MES Input File YouTube Video**

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In this video, I’m going to walk you through how to prepare an input file for the Magma Chamber Simulator. We’re going to prepare an input file for a fractional crystallization run, so if you need to prepare one for a more complex run, such as an AFC, RFC, or RAFC run, those will be covered in later tutorials. If you have not already installed the Magma Chamber Simulator on your system, please close out this video and refer to our other tutorial on installation of the MCS and its folder structure.

**0:29**

So the first thing we need to do is open up the input file. In order to get to that, we need to navigate to our Finder Window – again, if you’re not quite familiar with a Mac, that’s down here in the bar, and it’s the little happy face. From there, we can navigate to our Documents folder, and then into our MCS folder. Now our input files are located here, in this folder called “Input & Output”, and yours should come pre-loaded with some. You’ll notice that there is this general one at the bottom, and that’s called “Prototype MES”. That’s just a general input file that you can type over and use. But, because it does not begin with “MES\_”, it actually won’t pop up when you’re running the Magma Chamber Simulator, so it’s not an option to use. So that’s the file where you can input your own information if you want to make your own MES files. But for right now, we do have some pre-loaded for you, and we’re going to open up this one called “MES\_FC\_1”.

**1:34**

And I’ll go through and explain the different parts of the file (so let me zoom in here just a bit, so you can better see what’s going on). So the different regions of the input file are coded by color. Ttis blue box is the first one, and this contains our global system variables. The Magma Chamber Simulator is made up of three subsystems – the magma subsystem, the wallrock subsystem, and the recharge subsystem. Each has its own separate input, but these systems in the blue box – these are system variables that apply across all three subsystems, so we’re going to set them first.

**2:15**

The first global parameter we have here is in Row 2, and it’s called FmZero. This is the minimum mass fraction of liquid that must accumulate in the wallrock subsystem in order to trigger assimilation. Since we don’t want any assimilation to occur in this run, we can go ahead and set this value to 1. Essentially, what this is doing is telling the Magma Chamber Simulator that it has to melt 100% of the wallrock before assimilation can be triggered – and we know this is unrealistic; we’re never going to have enough heat for that to happen, so it’s a surefire way to turn assimilation off.

**2:50**

The next global parameter we have are the Excluded Phases: these are, as the name implies, phases that are excluded from all three subsystems. Now, an easy way to input these excluded phases is to do it actually directly from the Magma Chamber Simulator. So in order to do that, we can go ahead navigate back to our Documents folder, into the MCS folder structure, and we need to navigate back to this MCS VBL Code folder, and open up our MCS file – uh, remember, that’s this “MCS\_PhaseEQ\_2019 whatever version you may have”. So once we open up the MCS, remember we need to enable macros, and then we’re going to need to route Excel to the MCS folder structure before we can actually get to using the interface.

**3:57**

So we want to get to that bottom button here that says “Excluded Phase Help”. If we click on this, it brings up this user form, and that has a list of different mineral phases that can be excluded. So, for example, if I wanted to exclude spinel and tridymite from all three subsystems during my run, I could click here on “spinel”, and click the “tridymite” box as well. Then I click the “Copy to Clipboard” button. This automatically closes the user form, and you can exit out of the Magma Chamber Simulator – so remember, don’t save it! And now, we’re back to our MES file. Click on cell B3, and I usually right-click and I “Paste Special”, uh, just to paste those excluded phases in. So, I want to avoid any sort of formatting issues that might occur if I were to just Ctrl-V. Now, you can also type these in by hand, but by using this function on the Magma Chamber Simulator interface, uh, you can make sure that you don’t have any typing errors; this can also be helpful if you’re not sure what the different phases are that are available to be crystallized out in MELTS or the Magma Chamber Simulator. So, if you’d like to type the phases in by hand, you’ll notice that (1) they’re all in lowercase, (2) they also must be spelled correctly, and (3) if you’re excluding more than one phase, they must be separated by this carrot symbol, without any spaces. If these criteria are not met, the Magma Chamber Simulator won’t be able to recognize the excluded phases, and they won’t be excluded from your run.

**5:35**

The third parameter is pressure, and that’s given here in bars – it’s fairly self-explanatory. So I want to run my model at 1.5 kilobar – again, because MELTS takes in pressure in bars, so does the Magma Chamber Simulator. So I need to type in “1500 bars” in cell B4. Now you’ll notice that I’m not touching anything in column A or column D - those need to be left the way that they are. The Magma Chamber Simulator will actually read the text in columns A and D, so make sure that when you’re changing values in these input files, you’re only changing values in column B, or F and beyond. Columns A, C, D, and E must be left absolutely alone.

**6:21**

The next global parameter is labeled “Enthalpy Convergence Steps”. This is the number of steps that occur in an isenthalpic calculation, and those calculations only occur when other magmatic processes are modeled in addition to fractional crystallization. But, the Magma Chamber Simulator still does need a value for this, so let’s leave it at 30. You can set this parameter anywhere from 10 to 100, but through rigorous testing, we found that the sweet spot is 30 enthalpy convergence steps. So I would really just recommend sticking with that value, unless you really feel a need to change it.

**6:54**

Our final global system parameter is oxygen fugacity – that’s a measure of the redox conditions in the system. And you’ll notice that over here in column F (uh, let me scroll over and) there are a couple helpful hints here (alright, expand that a little bit). So, in Column F, for each row, we do have helpful hints listed – if you’re not quite sure what needs to go in where, and you don’t care to go back through this entire video. So here in column F – in cell F6 – we have the acceptable standard input values for the different oxygen fugacity buffers that are available in standalone rhyolite-MELTS. Because the Magma Chamber Simulator is built upon rhyolite-MELTS, we employ the same standard buffers. And so, we can choose between “none”, “QFM”, “Ni-NiO”, “IW”, and so forth. But again, they need to be spelled exactly as they are given here – all in lowercase, and in the case of “QFM”, MELTS has it listed as “FMQ”, so we need to type in “FMQ” if we’re going to be employing that particular oxygen fugacity buffer. But for this run, we want to run at the Ni-NiO buffer, so instead we’re going to type “nno” into this cell. And again, if it’s not input exactly as given in cell F6, the Magma Chamber Simulator will not be able to interpret the input file, and so it won’t be able to complete the run.

**8:31**

So now that we’ve covered our global system variables, we can move on the Magma subsystem – and that’s given here, next, in the green box. Our major oxides are listed in the same order as they are in standalone-MELTS, so this format should be pretty familiar already. And, just like in standalone MELTS, we want to make sure that our hydrous compositions are normalized to 100 prior to a simulation. I generally do this in standalone MELTS, just because I like to constrain the liquidus and solidus temperatures for each subsystem before I even put my input file together, but of course this can be done in Excel as well. You’ll notice that to the right we have this renormalization schematic over here in columns F and G. So if you put in some value in column F, it will come out in column G renormalized. For example, if I were to change the wt.% of water in this composition to 2, you’ll notice that I get a new output composition, renormalized to 100 wt.% in column G. Uh, now after you’ve renormalized your composition – if you don’t use standalone MELTS to renormalize – you can just copy these values and then paste them, because these are kept in the same order. And again, I like to “paste special”, and then paste the values – just to avoid any sort of possible confusion in Excel with formatting (we can undo that).

**10:00**

And now, after we’ve input our starting composition for the magma, the next parameter we have is the starting temperature, and that’s here under “Tstart”. It doesn’t really matter what we put in here, because the Magma Chamber Simulator will always start at the liquidus. But, I like to help the MCS out a bit and give it a temperature that I think is reasonably close to where the liquidus might be, just to give it a better jumping-off point from its initial guess. Again, if you’re unsure what a reasonable liquidus and solidus temperature are for each of your compositions, I would highly recommend running each of them through standalone MELTS just to get those values first. I find that although doing this is an extra step, it will avoid having to redo a lot of runs because perhaps your composition isn’t quite right, or you’re not really sure what the solidus temperature for the wallrock would be. Now, of course, you could just do an FC-only run in standalone MELTS, but we are going to do it in MCS because the Phase Equilibria output file for this is the input file for the MCS Trace Elements Engine – and that’s really very useful.

**11:01**

The next parameter in our Magma subsystem is our temperature decrement, or delta T. That’s gonna be in cell B30. This is the number of degrees in between each equilibration step in the run. So, for example, let’s say that the liquidus temperature for a composition is 1050 degrees, if my delta T is 20, the next equilibration step that is output will occur when the magma composition is at 1030 degrees. And after that, the magma composition will cool another 20 degrees to the next equilibration temperature of 1010 degrees, and so on and so forth.

**11:36**

So in the Magma Chamber Simulator, the end of a run occurs when the magma and wallrock subsystems reach thermal equilibration. Depending on your starting masses, compositions, temperature, the set deltaT, and many other parameters you choose, this can have the capacity to take a really, really, really long time. And if you’re not in need of data at temperatures near the magma-wallrock equilibration temperature, you can use these Hard Stop functions we’ve added here in Rows 31 and 32, in order to terminate the runs prematurely. So say maybe I’m only interested in olivine fractionation, or other high-temperature processes, and I’m not concerned with things that are happening near the solidus of this composition, I could stop the run at, say, 850 degrees. And what will happen is when the Magma composition drops to any temperature lower than 850 degrees, the run will completely terminate.

**12:27**

Now, in addition to setting this “Hard Stop Temperature”, the newest version of the Magma Chamber Simulator also has this “Hard Stop Melt Mass in the Magma”. This is the Magma Chamber Simulator stopping when the mass of liquid in the Magma subsystem reaches some number of grams. Now, because there’s 100 grams initially in the subsystem, we can think of this sort of as a percentage. So if you wanted to terminate the run when there’s 6% melt in your magma left, you can put “6 grams”, and that will stop when there’s 6 grams of melt left in the Magma subsystem. And that wraps up our magma subsystem parameters.

**13:03**

So what’s really nice about this newest version of the Magma Chamber Simulator is that if you are only interested in doing fractional crystallization, at this point we’ve completed our input file. We can leave the pre-populated values in the rest of the boxes, because MCS now has a workaround for the wallrock prime step. We don’t need to be concerned about what’s in the wallrock composition, or in the recharge composition, uh, because the Magma Chamber Simulator doesn’t even actually consider it – it will know that you don’t want assimilation. So again, if you’re not doing anything with assimilation, you don’t need to perform the “wallrock prime” step, and you don’t need to fill out anything further. Uh, but, if you do need information on the wallrock subsystem, you will need to perform that prime step; we’ll address that or do that in later tutorials that concern assimilation.

**13:56**

So we can go ahead and close this out, but before we do, don’t forget to save your Input file! MES Files will need to be saved in this “Input & Output” folder – so we can go ahead and “Save As”, and just to save it as something else, we’ll call it “MES\_FC\_2”. So, that concludes our tutorial on how to prepare an MES input file for a fractional crystsallization-only run using the Magma Chamber Simulator. In our next tutorial, we’ll actually use the Magma Chamber Simulator to perform this FC-only run.

**14:39**