**Transcript of MCS v.2019 MCS Traces & Isotopes Save to PAR File Tutorial**

**0:00**

The newest feature of the Magma Chamber Simulator is its ability to now model trace element and isotopic behavior, according to the major oxide phase equilibria results. In this tutorial, I’ll introduce you to the MCS Traces interface. Let’s navigate to our MCS folder structure, and we’re going to want to open up the MCS VBL Code Folder. A quick warning – *if you have not yet installed the Phase Equilibria part of MCS, do not open either Trace Element File* – this can cause installation issues. Also, you need to run the main MCS anyways, because MCS Traces takes the output file that’s generated by MCS Phase Equilibra, and actually uses it to perform the trace element calculations. In the MCS VBL Code Folder, we have our MCS Phase Equilibria file, and then we have two other Excel files: the “MCS\_TE\_Engine”, and “MCS\_TraceElement\_Isotopes\_2019{ver}”. “MCS\_TE\_Engine.xlsx” is the actual Trace Elements engine that performs the calculations, and “MCS\_TraceElement\_Isotopes\_2019{ver}” is the user interface for the engine. You want to leave the “MCS\_TE\_Engine” file in this folder so that the MCS can access it, but you do *not* want to open it. If the Trace Elements Engine is open when you start a run, MCS will not operate properly – so, just keep the file in the folder, keep it closed and leave it well enough alone. But for now we can open up the MCS Trace Element Isotope file.

**1:35**

Just like MCS Phase Equilibria is an Excel macro, MCS Traces is also an Excel macro, so once we open up the file, we’re going to need to click “Enable Macros”. The next pop-up box tells us which version of MCS Traces and Excel we’re running (we can click “OK” to get rid of that box…), and we’re going to need to allow Excel to communicate with the MCS Folder Structure, so just like with MCS Phase Equilibria, we need to click “OK”, make sure that the MCS Folder is here selected at the top of the window, and click on “Choose”. The MCS Traces interface is similar to the MCS PhaseEQ interface – in that we can start at the top, and end up working our way down to the bottom.

**2:19**

The first thing we want to do is select which MCS Phase Equilibria Output File we want to model trace elements and/or isotopes for. Click on the top button to bring up a user form where you’ll be able to select which one you’d like to use – in this case, we can click on the arrow to bring down the drop-down menu, and we want to select our Output File from the RFC byTemp run that we did earlier, and then click finish. Just like with MCS Phase Equilibria (if you were watching…) you should see that text has been changing in the bottom, lower left corner of the Excel workbook. So, if you’re not sure what steps you should take next, or if you’re not sure whether or not the MCS is frozen, keep an eye on that bottom left-hand corner to make sure that text is changing.

**3:15**

Our next step is to pick the Trace Elements we want to model, so we can click on the next button, and a periodic table will appear in a new tab. I really appreciate the ease of the user interface here – MCS Traces is pretty intuitive to use, as geochemical modeling software goes. And, as you can see, some of the elements on the periodic table are greyed out – these symbols are either major oxides (so they’ve already been modeled using MCS Phase Equilibria), uh… they could be not very commonly used trace elements, or they’ve not yet been activated in MCS Traces. But, we do have a plethora of elements to choose from – we could even choose all of them if we wanted to, by clicking on “Activate All”. Once I do that, every element that is selected to be modeled will have chevron symbols surrounding it. If there are elements selected that you do not wish to model, you can deselect that element by clicking on its symbol, like this. We can also use the “Deactivate All” button to clear all of the elements out. And, after you’ve done your first MCS Traces run, if you have a standardized set of trace elements that you like to use, you can click on “Load Previous Selection”, and it will bring up the set of trace elements that were modeled on the last run.

**4:35**

The last restriction on which elements can be modeled applies primarily to those minor elements which are included in standalone r-MELTS as potential inputs – so, elements like Ni, Co, and Ti. In the MCS Phase Equilibria part of your run, if you have modeled these elements and try to select them as a trace element as well, MCS will not allow it, and you’ll get this pop-up box here telling you so. But, for this example, I only want to model a few elements, so we can “Deactivate All”; let’s select Sr, O, and Ni – you’ll see why I’ve selected those three particular elements shortly. In order to get back to the main page of MCS Traces, we can select “Back to Main Menu”, and here we are. Now that we’ve selected which elements you’d like to model, we need to set the initial concentrations of the trace elements, and their partition coefficients. Let’s click on the first button in our 3rd row: “Set Initial Magma TE Concentrations, Initial Isotope Ratios and Solid/Melt Partition Coefficients”, and we’re brought to a new worksheet where we can input these parameters.

**5:47**

The Magma Subsystem worksheet is divided into two sides: initial concentrations are to the left of the yellow column, and mineral-melt partition coefficients to the right. The first column is a list of the trace elements you’ve selected to model, and then their initial concentrations (in ppm) for the Magma Subsystem need to be entered in the next column, Column C. The first time you do a run in MCS Traces, you will see lots of large, random, unreasonable numbers here. This is just a default setting because Excel required some random numbers to be generated… and you’re going to go ahead and change these when you set up your run, so don’t worry about it. In my Magma composition, I should have 92 ppm Ni, and 408 ppm Sr, so I have those values in the appropriate rows. I also have initial isotope ratios to put in, and isotope ratios go in Column D. So I have my Sr isotope ratio, and then my δ18O value is gonna go here, in the red box. You don’t need to input a concentration for O, but in order to calculation the O-isotopes, you do need to input the δ18O value.

**6:59**

On the right side of the worksheet, you’ll find several columns of data – each mineral phase that is fractionated out during the run will be present here. Mineral-melt partition coefficients for each element modeled for each mineral phase that is fractionated will need to be input in these cells; and you can get these from the GERM KD database (that’s located online at <https://earthref.org/KDD/>). And we don’t have any KD values for O, so that row’s gonna stay blank – the only thing that should have any data in the O row is the δ18O value. BUT, we can put in partition coefficients for Sr and Ni for each mineral phase in this run., which I’ve input. After we’ve put in the mineral-melt partition coefficients, we want to click the button that says “Go to Next”.

**7:56**

MCS Traces does consider KDs for any exsolved fluid phase present in the run, and since fluids in MELTS can now consist of both H2O and CO2, we’re going to need to input mineral-fluid partition coefficients for both H2O and CO2. If you don’t want to consider the fluid phase in the trace elements modeling (like I very rarely do), I set these to 10,000 – so remember, these are **solid-fluid** partition coefficients, so we want the numbers to be big to avoid having our trace elements partition into the fluid phase. After you have done this, click the “Go to Next” button again – we need to do the exact same thing with the solid-fluid partition coefficients, but this time we have CO2 as the exsolved fluid phase instead of H2O. So pretty much unless you are actually wanting to model how the exsolved fluids affect your trace elements, set all of these values at 10,000. Otherwise, you should put in the appropriate partition coefficients for your particular modeling scenario, and treat the exsolved fluid phase no differently than you would any other mineral phase. Once we have our mineral-melt and mineral-fluid partition coefficients set for the Magma Subsystem, we want to click on “Back to Main Menu”.

**9:19**

Now we need to set the same parameters for our Recharge Subsystems. In this run, we have two separate recharge events, indicated by the two different buttons that read “Set TE Conc & Isotope Ratios for Recharge Event”. I also appreciate how the button will specify which “Recharge Event” you have assigned it when we first made our MES Input File, as well as the specific conditions for each recharge event. This is really helpful for keeping your multiple recharge events straight! For each separate recharge event within a model, you will need to input its respective initial concentrations and isotope ratios. We can click on the button for the first recharge event. And notice how unlike the Magma Subsystem, we don’t have any place to put partition coefficients here – that’s because we have a single equilibration step for each Recharge event, and no fractionation takes place during that step. So we just need to input our initial Ni and Sr concentrations, our Sr isotope ratio, and our δ18O value. Clicking the “Go to Next” button will take us to the second Recharge Event and we can input the initial trace element and isotope values for Recharge 2 here. Once we have completed this step for each recharge event, we’re almost ready to let MCS take the wheel. So let’s click on “Back to Main Menu” to navigate to the main MCS Traces page.

**10:45**

Now before we actually run the calculation, it might be nice to save the input parameters we have for this run. This way if you have to redo it, or if you have a similar run with slightly different parameters, you don’t have to go through these steps every single time, because that would be the *absolute worst*. Let’s save our Magma and Recharge initial concentrations, as well as the partition coefficients that we’ve assigned, so that we can use them again in another run. Click on the button labeled “Load or Save Partition Coefficients, Concentrations and Isotopes from saved PAR files”. In the next tutorial, we’ll work through an AFC Traces file involving the Wallrock Subsystem, and I’ll show you how to do this working from a PAR file you’ve already saved. But in the meantime, we’re going to create a new PAR file. Your filename must be 20 characters or less, without spaces. So let’s name this “Traces\_Example1”, and click on “Save to PAR file”. Now, MCS might take a minute or so to create the PAR file – again, you want look down here in the bottom left-hand corner of the Excel window to make sure that it’s not frozen. Once the PAR file is created, click “OK” to return to the main MCS Traces interface. PAR files will be automatically saved to the “Input & Output” folder within the MCS folder structure, into this “PAR Files” folder. Once it’s been created, you can go into the folder and rename it to anything else you’d like… uh… But, otherwise, we have finished preparing the input parameters for our MCS Traces run.

**12:47**

The final button on the MCS main Traces interface is the button that actually performs the Trace Element Calculation. Once you press this button, **let go of the mouse**. This is gonna take a little while – uh, the more elements, mineral phases, and temperature steps your model has, the longer this calculation will take. So for those longer runs, I may go run a quick errand or go do something else, and come back to the Magma Chamber Simulator. When it says “Long Wait”, it means “Long Wait”.

**14:22**

Alrighty! Once the calculation has finished, the results are automatically saved as new sheets in your MCS Output File. We can click OK, and now we’re back to the main MCS Traces interface again. If you have multiple trace element models to calculate, you can actually go ahead and start all over again without exiting out of Excel – unlike the Phase Equilibria part of MCS, uh, Traces doesn’t require that you exit out of the macro workbook and re-open it before doing a new run – you can leave it open and do several in a row, which is really nice. But, I do find that this tends to make the Magma Chamber Simulator a bit sluggish if you do it too many times, so I generally exit out of Traces and restart it about every 10th run or so, just to keep things running smoothly. If you don’t have any other Trace Element models to run, you can close out MCS Traces – and remember, **do not save the file**.

**15:22**

The results of our Trace Elements model have automatically been appended to the beginning of our original MCS Output File, RFC\_byTemp. MCS Traces will automatically save your data, but I like to do it again (just because I’m a wee bit paranoid). So this concludes our first tutorial on the MCS Trace Element & Isotope Calculator. In later tutorials, I’ll show you how to do a Trace Elements AFC run from a pre-populated PAR file, and we’ll talk about how to read the Trace Element output results.

**15:55**