

READING MCS OUTPUT FILE

After a successful simulation, click EXPORT RUN RESULTS (Step 5) from the MCS interface. Then open up the MCS folder and open the INPUT & OUTPUT folder. The name of the OUTPUT is whatever you assigned during run setup. It is a six-character file name with extension .XLSX. Here we will review the different tabs and columns of this user-named output file. This is where the results of the simulation as well as an echo of the input (the MES_*filename*) is located. When you open the output file you will note that it has a number of tabs. The text below explains the information of each sheet.

“Input” tab:

This tab mostly echoes the information from the input file (MES file). Therefore, we will not review this here; it is explained in the description of the MES file available by clicking SETTING UP MES INPUT <MES_*filename*> button. One element provided is the identity of the computational MELTS engine utilized. This is important information that you should remember to report together with the results of your run in any publication since the engine version is required for reproducibility by another researcher.

“RunSummary” tab:

This is the most important tab of your output file as it contains information about the changes in mass, phase equilibria, temperature, and chemistry within the modeled system. We will thus review most of the columns in detail here.

Column B, “Melts Run Mode”:

Provides information on the processes that take place in the system at a given temperature or during a given temperature step.

“WallrockPrimeSupra” = This is the state of Wallrock at the temperature (T) where the melt fraction equals the user-input fmzero value as found during “Find Wallrock Solidus” calculation. This is not yet part of any temperature step of the MCS model *per se*. Row 4 gives complete state of the Wallrock subsystem at the T where the fraction of melt in WR equals fmzero: amount and composition of all phases including the liquid composition. Recall that when the local melt fraction in WR exceeds fmzero, then partial melts from WR will be transferred across the WR/M interface (i.e., added to the M sub-system).

“MagmaFindLiquidus” = Initial (liquidus) T of M parental magma appears only on row 5. Note that this is the T at which the first *SOLID* appears. If the M parental magma is saturated with H₂O (v.1.0.2 or pMELTS) or fluid (H₂O-CO₂ in 1.1.0 or 1.2.0) this is considered the liquidus phase for this operation in MCS. MCS simulations start at the T of M magma where the first crystal precipitates.

“MagmaEquilibrateB” = Equilibrium crystallization in the melt in the magma chamber within one temperature step. Remember that solids are removed afterwards and thus fractionation takes place after each step.

“RechargeEquilibrate” = State of recharge magma at the time of recharge *before* addition to M sub-system

“MagmaEquilibrateC” = Equilibrium crystallization one temperature step *after* recharge has taken place. Remember that fractionation takes place after each step. To monitor the effects of recharge, an isenthalpic step, the output of this operation gives the new magma T, mass, amount of solids removed and M melt composition. Scroll to the right and find the information you require.

“WallrockEquilibrate” = State of the wallrock at a given temperature.

“WallrockChangeBulk” = Extraction of melt from the wallrock at a given temperature. This gives the state of the WR system including the amount of partial melt that WR has given up to M sub-system.

“MagmaIsoTFractionateB” = State of M subsystem after to the mixing of the wallrock partial melt into it and full equilibration.

Columns C–F, “Magma Chamber Process” column and temperature columns (in blue):
Rather self-explanatory, refer to the explanations of the “Melts Run Mode” column.

Column G, “Total Composite System Mass (grams):

Gives the total mass of the system. The mass of the initial magma is always 100 units of MCS mass. It is convenient to consider that the M magma starts at 100 g although one can consider this to be 100 kg or one ton! Masses can be scaled anyway one chooses. The first number in this column is the sum of all composite system masses in MCS mass units. Mass of a recharge magma is added to this number after a recharge step.

Column H, “Magma Liquid Mass (grams)”:

The mass of liquid in the magma chamber. It decreases by crystallization and increases by addition of recharge or wallrock melt. It does not include the fraction of melt that remains in the wallrock after each “WallrockChangeBulk” step (this fraction, FmZero, has been pre-defined by the user in the MES_ *filename*).

Columns I–L, Incremental and total crystal and fluid masses removed from the magma:

The mass of crystal cumulates and fluids removed from the equilibrium system after a particular step, and their total mass throughout the run. Fluid is pure H₂O (when using MELTS engine v1.0.2 or pMELTS) or H₂O-CO₂ mixture (when using MELTS engine v.1.2.0 or v.1.1.0). If the system does not contain a separate fluid phase as defined by MELTS algorithms, columns “K” and “L” will give zeros.

Columns M–P, The state of the recharge magma before addition of R to M. The internal state of R magma is given *before* addition to M. If the user-defined temperature of the recharge magma is below its liquidus temperature and/or volatile-saturated, recharge magma will contain crystals and fluid (H₂O or H₂O-CO₂ mixture) and details on the amount and composition of all phases is given. As MCS models equilibrium systems

only, upon mixing antecrysts in R and vapor bubbles are equilibrated in the new magma whose bulk composition is equal to old M magma plus the Recharge magma, appropriately weighted by mass. The hybrid magma is an equilibrium magma: nonequilibrium is not allowed. The following “MagmaEquilibrateC” step then calculates the first equilibrium crystallization step after such recharge. In cases where crystal-rich recharge magma was injected, the mass of crystals forming in column “I” in “MagmaEquilibrateC” step may be rather large.

Columns Q–V, The state of wallrock:

“Wallrock Subsystem Mass (grams)” = The mass of wallrock that has not yet melted and hence remains in WR. Every time a portion of wallrock partial melt is mixed into the magma chamber, this mass decreases by that amount.

“Wallrock Subsystem Residual Liquid Mass” = The mass of wallrock melt that is not mixed into the magma chamber, but remains in the wallrock in equilibrium with the residual solids (+ fluids). This is defined by the FmZero value in the MES input. For example, if FmZero is 0.1, this number is 10% from the number in the previous column (if the mass of wallrock melt in total is above 10%).

“Wallrock Subsystem Solid (Crystal) Mass” = The mass of residual solids remaining in the wallrock.

“Wallrock Subsystem Residual Fluid Mass” = The mass of residual fluids remaining in the wallrock.

“Incremental WR Liquid Added to Magma (grams)” = The mass of wallrock partial melt that is above the user-defined FmZero fraction and is mixed into M sub-system during this step.

“Cumulative WR Liquid Added to Magma (grams)” = The cumulative mass of wallrock melt that has been mixed into M.

Cyan columns, Magma mineral phases (incremental and total):

These columns list the masses of all phases that were present in the magma chamber in equilibrium with a specific melt composition at the end of a temperature step (incremental) and their total masses in the cumulate pile (total). The sums of incremental and total crystals should equal the masses in columns “I” and “J”, respectively. The phases are defined by MELTS algorithms and it is important to note that because of that, there may be several different clinopyroxenes, feldspars, etc. listed here. This is related to how MELTS treats solid-solutions: for example, feldspar {1} corresponds to plagioclase whereas feldspar {2} corresponds to alkali feldspar component. User can find the exact compositions of these phases after each step in the “SolidFormulas” tab. Negative values may also occur in the incremental columns, for example, in cases where a phase is at the cusp of instability. These are also related to how MELTS uses so-called seed crystals for calculating stabilities of different phases and are nothing to be worried about (negative number indicates that there was not enough seed mass to form actual crystals). These negative numbers are usually in milligrams, and do not have a significant effect on the total mass of the crystals or the system as a whole. Simply ignore the tiny negative mass increments: they are an artifact of the numerical method used to compute the stable assemblage

Blue columns, Recharge magma mineral phases (incremental and total):

If the recharge magma contained crystals during the time of injection, this is the crystal assemblage and masses of each phase in it. The masses of these crystals should equal the mass in column “O”. As mentioned earlier, all of these crystals are mixed into the magma chamber.

Green columns, Wallrock mineral phases (incremental and total):

The mineral phases present in the wallrock in the end of a given temperature step. The sum of these phases should equal the mass given in column “S”. The minerals are in equilibrium with residual liquid and fluid phases, the masses of which are given in columns “R” and “T”, respectively. Note that when the melting of the wallrock proceeds, the mineral composition of the wallrock becomes more refractory (i.e. more mafic).

Gray columns, Magma melt chemical composition:

The composition of the melt in the magma chamber. Note the effects of mixing with wallrock partial melt or recharge melt. Remember that this composition does not include the separate mineral (+fluid) phases.

White columns, Recharge magma melt chemical composition:

The composition of the recharge melt in the time of recharge. Note that if your recharge magma contains crystals or fluids, the masses of which are given in columns “O” and “P”, they are not included and the composition is then different from the one that you gave in the MES input.

Gray columns, Wallrock melt chemical composition:

The composition of the wallrock melt in the wallrock. This is both the composition of the wallrock melt that is mixed into the magma chamber (mass defined in column “U”) and the melt that is left behind because at any given step these compositions are necessarily identical (mass defined in column “R”).

“Charts” tab:

Displays the charts the user defined to be displayed in the MES input file.

“SolidFormulas” tab:

Here you can find the chemical compositions (formulas) of each mineral phase calculated to be in equilibrium in the wallrock, recharge melt, or melt in the magma chamber in the end of any temperature step. It starts with wallrock equilibration (“WallrockFindSolidus” and “WallrockPrimeSupra”), after which the phases of the actual MCS run are listed for every temperature step.

“XChartData” tab:

Numerical information for the “Charts” tab.