

## Setting up MES Input: the <MES\_filename> file

The MES spreadsheet contains the input for all parameters required to run a Magma Chamber Simulator (MCS) simulation.

### Columns:

Column A includes descriptions of the required input parameters

Column B includes the values of those parameters, most of which are entered by the user.

Column D includes names/strings of characters that are used by the computer code.

**Values in column D should not be modified.**

Column F includes comments that define or provide additional information about parameters in each row.

Column G, rows 9-26, 33-49, 64-81, 91-108, 118-135, 146-162, and 172-189 represent values in column F that have been normalized to 100%. Enter the relevant value into the cell in column F, and then copy the normalized values into relevant cells in column B. Further instructions provided below.

### Rows:

SYSTEM VARIABLES (rows 2-6): these parameters, which apply to the entire composite system (melt, crystals, wallrock, recharge reservoir(s)), are as follows:

Variable Name (Column A)	Definition/Explanation	Example Value
Fmzero (wallrock) (fraction) (row 2)	Minimum wallrock (WR) melt mass fraction to trigger addition of anatectic melt from WR to M (Magma) subsystem. For each occurrence when anatectic melt is transferred to M, the WR melt fraction (after transfer) is equal to fmzero. Based on rheological studies, fmzero may typically lie in range 0.01 to 0.15.	0.05
Excluded Phases (row 3)	This feature allows the user to exclude phases from a simulation. Using the MCS interface, click "Help for Excluded Phase", click on phases you wish to exclude, press put in clipboard, and paste in column b, row 3. The phases excluded will be excluded in all three subsystems WR, M and R.	
System Pressure (in bars) (row 4)	Simulation is isobaric; chosen pressure (in bars) applies to M, WR and Recharge (R) subsystems.	1000
Enthalpy Convergence steps (row 5)	During Assimilation (A) and R steps, thermodynamic isenthalpic calculations are performed. During these calculations, the system enthalpy rather than temperature is incremented from an initial to final state. The value entered here controls the size of the increment. This value should be a positive nonzero integer. An operational range is circa 5-100. A typical value is 30. EnthConvergenceSteps has no effect on the solution although a poor choice may prevent a solution from being attained. Set at 30 and change only if system crashes during AFC or R operation or if very large or very small amount of A or R is added to M subsystem.	30
Oxygen fugacity (row 6)	Acceptable input values are: none, fmq, coh, nno, iw, hm. Input these exact strings of characters. These are standard oxygen buffers. When choosing 'none' be sure to input reasonable values	none

	for Fe <sub>2</sub> O <sub>3</sub> and FeO into M, WR and R compositions. For many applications setting 'none' and then making FeO 80 to 85% of the total iron oxide (FeO <sub>T</sub> ) is suggested.	
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M Composition (wt%) (rows 9-27): weight percent (wt. %) oxide initial values for M. Values in these rows should sum to 100%. To normalize values to 100%, enter values in rows in column F, and then cut and paste values in column G into column B. Note that some values (SO<sub>3</sub>, Cl<sub>2</sub>O and F<sub>2</sub>O) are listed but cannot be input into the current version of MCS.

Temperature start (°C) (row 29): temperature at which the magma "Find Liquidus" operation begins. Once a liquidus temperature is established, the MCS simulation commences.

Temperature decrement (°C) (row 30): a positive number reflecting the temperature decrement for the cooling magma body, M. Typical values are 5-20°C. For reconnaissance work, 30-50 °C can be used. Temperature decrements of <1°C can be unstable and should not be employed.

Hard Stop Temperature (°C) (row 31): when the M temperature reaches the hard stop temperature, the simulation ceases. A nonzero value is typically used when running fractional crystallization (FC) or recharge (RFC) simulations. Otherwise, zero (0) should be used.

WR Composition (wt%) (rows 34-52): weight percent (wt. %) oxide initial values for WR. Values in these rows should sum to 100%. To normalize values to 100%, enter values in rows in column F, and then cut and paste values in column G into column B. Note that some values (SO<sub>3</sub>, Cl<sub>2</sub>O and F<sub>2</sub>O) are listed but cannot be input into the current version of MCS.

INITIAL WALLROCK TEMPERATURE AND MASS (rows 55-59): these parameters are as follows:

<b>Variable Name (Column A)</b>	<b>Definition/Explanation</b>	<b>Example Value</b>
Wallrock find solidus: end temperature (°C)	Every MCS simulation must run the routine " <i>Find Wallrock Solidus</i> ." This value represents the Ending temperature of the WR "Find Solidus" routine. This temperature should be set to ~10 degrees below the solidus of the WR composition. If set too low, the phase equilibria engine may not be able to return a solution. We recommend using MELTS done in equilibrium crystallization mode to determine the solidus temperature, and use the determined solidus temperature to inform the choice of end temperature.	850
Wallrock find solidus: temperature (°C) decrement	Positive number reflecting temperature decrement for the <i>Find Wallrock Solidus</i> routine.	5
Wallrock find solidus: start temperature (°C)	Starting temperature for <i>Find Wallrock Solidus routine</i> . WE recommend, based on MELTS run noted above, to choose a temperature that yields 40-50% melt. Note that the start temperature does not need to be the liquidus temperature.	1050

Initial Wallrock Solid Mass (grams)	All MCS simulations start with 100 grams of M magma. The initial wallrock solid mass is the mass that thermally interacts with M magma. E.g., if WR initial mass =100 (grams), then during MCS simulation, heat extracted from M is added to 100 grams of WR. If initial wallrock solid mass is 150 (grams), then the heat derived by cooling and crystallization of M will be added to 150 grams of WR.	100
Wallrock Initial Temperature (°C)	Initial temperature of wallrock subsystem at the start of the simulation.	650

RECHARGE General (row 61): sets mode for addition of recharge magma. Applies to all recharge events in simulation.

Recharge Trigger Mode (byDelta OR byTemp) (row 62): only acceptable entries are *byTemp* or *byDelta* (case sensitive).

When using *byTemp*, recharge addition occurs when the magma temperature attains the value set in rows 88, 115, 142, 169, and 196 (for the five recharge events). For example, if *byTemp* for the first recharge event is 1150°C, then magma cools from its liquidus (e.g., 1200°C) to this prescribed temperature (1150°C); when this magma T is reached, the recharge mass is added. The next recharge event (RECHARGE EVENT 2) requires a M temperature (when recharge occurs) that is lower than event 1 (e.g., 1100°C). Lower magma temperatures are then required for recharge events 3, 4, and 5.

When using *byDelta*, recharge addition occurs when the magma temperature has decreased by this value from the magma liquidus temperature. For example, if magma cools from its liquidus (e.g., 1200°C) and the *byDelta* value (in row 89) is 30, then recharge mass will be added when magma temperature reaches 1170°C. In this case (for example), the new hybrid magma temperature is 1220°C (i.e., after the mixing event). If the next *byDelta* (row 116 for recharge event 2) is 50°C, then recharge magma is added when the hybrid magma drops 50°C to 1170°C. Each relevant recharge event requires an entry in the relevant cell in column B, and the delta temperature increments can be different but all must be positive.

RECHARGE EVENT 1 (wt%) (row 64):

Rows 65-83: these are weight percent (wt. %) oxide values for the first recharge subsystem.

RECHARGE EVENT 1: TEMPERATURES AND MASS (row 85):

Recharge Event 1: Mass (grams) (row 86): this value is the mass of recharge magma added during Recharge event 1. For example, if 50, then the ratio of mass of recharge magma to initial mass of M is 1/2 (50/100). If this mass = 0, no recharge will occur. (recall that by default, the initial magma mass is always 100 grams).

Recharge EVENT 1: R Magma Temperature (°C) (row 87): the temperature of recharge magma when the recharge event occurs (i.e., recharge magma is added to M). The recharge magma temperature determines the state (melt±crystals±volatile phase) of this magma when recharge occurs.

Recharge EVENT 1: when byTemp: temp (°C) of M magma at recharge instant (row 88): Temperature of M when recharge magma is added to M. Ignored when TriggerMode (row 62) is set to byDelta.

Recharge EVENT 1: when byDelta: delta temp (°C) of M magma at recharge instant (row 89): temperature decrement (set as positive number) from magma liquidus temperature at which the recharge magma will be added. Ignored when TriggerMode is set to byTemp.

RECHARGE EVENTS 2, 3, 4, 5: OXIDES, (wt%) and TEMPERATURES AND MASS (rows 91-197): all parameters described above (rows 64-83 and 85-89) are similar for events recharge 2, 3, 4, and 5, with the exception of row 89. For recharge events 2, 3, 4, and 5, the delta temperature is decremented from the (newly calculated) temperature of the hybrid magma produced by the previous recharge/mixing event. See above explanation for byDelta for example.

GRAPHING (row 199)

Rows 200-201 (Graph 0 X axis, Graph 0 Y axis): these set the x and y axis for the wallrock find solidus results. Plots wallrock temperature (during Find Solidus operation) vs. wallrock %melt. **Do not change these entries.**

Rows 202-261: All X-Y pairs 1 thru 30 (e.g., Graph 1 X axis, Graph 1 Y axis): all entries require "Magma/" followed by one of the oxides (case sensitive) for both X and Y axes. Only oxides listed in MES file can be used (e.g., SiO<sub>2</sub>, FeO, etc.). Up to 30 graphs can be plotted. No oxides sums permitted; for example, if a TAS diagram is desired, data from the output must be copied into an Excel file and manipulated for graphing.

## **EXECUTABLES**

Rows 264-267: record of information from MELTS. **Do not alter these entries.**