

NOTES ON .tbl FILES AND ON TRACE ELEMENT MODELING

Note about the .tbl files

Along with the MCS run results, MELTS-produced "**phase.tbl**" files are generated in MAGMA, RECHARGE, and WALLROCK folders for each phase that is stable during the computation. For (well understood) computational reasons, the masses in the **.tbl** files do not exactly match the masses recorded in the RunSummary of the MCS output. In addition, for some phases (clinopyroxene is a good example) the excess Gibbs free energy model (i.e., the activity-composition relation for the crystalline solution) will (correctly) generate multiple phases. For instance, in slowly cooled rocks clinopyroxene can exsolve multiple distinct phases as exsolution lamella. *In MCS output, these are labeled as cpx{1}, cpx{2}, for example, and the .tbl file will have all cpx phases in a single .tbl table.* The user should beware of such idiosyncrasies if using the **.tbl** tables. In practice, the MCS team suggests **phase.tbl** files be used for gathering thermodynamic properties or mineral compositions on an oxide basis. These compositions are accurately linked to the temperatures in the **.tbl** file and are one-to-one with RunSummary results in MCS. *If user needs phase masses, the masses reported in RunSummary not in the .tbl files should be used.*

Note about sources of error in trace element modeling

Note that any possible negative solid and fluid masses ("seed crystals"; these are related to how MELTS algorithm performs the calculations) have been approximated as zero for the trace element calculations. This ensures that these very small negative masses do not cause negative trace element concentrations for those elements which have high K_{sm} or K_{sf} values. The effect of this approximation on the trace element model results was determined to be negligible (<0.1% difference in regards to total masses, i.e., less than the analytical error of any major and trace element geochemical data).

In addition to seed crystals, potential small error for trace element calculations may come from using fixed oxygen buffer. Because in such simulations the system is kept open for oxygen, the initial mass constraints used for the current trace element modeling code are not fixed throughout the simulation. In testing of reasonable simulations, we have found these errors to be generally less than 1% and thus similarly negligible. If modeling trace elements on simulations that use oxygen fugacities that cause significant changes in Fe_2O_3/FeO relative to the starting compositions (and thus in masses), we suggest checking that the total masses of the subsystems do not deviate more than 1% from the input values.

Note about solid-solutions and associated trace element modeling

In some runs, user will see multiple columns denoting distinct phase compositions for some solid solutions in the RunSummary of the MCS output. For instance, in slowly cooled rocks clinopyroxene can exsolve multiple distinct phases as exsolution lamella as the temperature drops. That is, at high temperature there is one and only one clinopyroxene but at some lower temperature two distinct clinopyroxene can coexist. The most common crystalline solutions where this phenomenon might appear are for clinopyroxene and feldspar. In **RunSummary** the distinct phases are separated from each other with suffixes {1}, {2}, and {3}. You may observe in some runs that the compositions of these distinct phases (these are listed in the **SolidFormulas** tab of the MCS output or in the **.tbl** files) do not always follow along with the numeral suffixes: e.g., if original clinopyroxene {1} ceases to crystallize, the original clinopyroxene {2} may take its place as the "new" clinopyroxene {1} for the remainder of the

run. This may become important for trace element modeling, since the trace element tool uses the columns from the RunSummary to distinguish different phases. For example, one could use a high partition coefficient (K_d) for Sr in feldspar {1} if its anorthitic in composition in the beginning, but if feldspar {1} is switched to sanidine composition in the middle of the run, the initially chosen K_d would not be optimal for the rest of the run. *Therefore one should always check the composition of a solid solution (e.g., {1}, {2}, etc.) in RunSummary before computing a trace element model to be sure that the choice of K_d is appropriate.* This is especially important for feldspars since the K_d in alkali feldspar solid solution (mainly NaAlSi₃O₈-KAlSi₃O₈ but with a small CaAl₂Si₂O₈ component) for some elements might be significantly different than the K_d of that same trace element in plagioclase solid solutions (mainly NaAlSi₃O₈-CaAl₂Si₂O₈ but with a small KAlSi₃O₈ component). In the future versions of the MCS package, the feldspar label convention will be made static such that feldspar{1} will always be plagioclase and feldspar{2} will always be alkali feldspar. In the meantime, when performing trace element modeling be aware that the feldspar labeling convention is dynamic and can change during a single simulation. Always check mineral composition using the formula tab to be sure. In the case of monoclinic pyroxenes, we recommend using uniform partition coefficients (K_d).