



List of files in this archive

Top level directory:

Note: All files except the executable are plain text (space delimited, no tabs).

Executable:

MCS_trace.exe (Windows), or MCS_trace (Linux)

Data input:

MCS.dat – must contain input temperatures and compositions. The supplied file includes all the compositions used in the examples in this document, expressed on both a molality (moles per kg of pure water) and amount content (moles per kg of solution) basis.

Results output:

MCS.rs1 – verbose output of all results.

MCS.rs2 – column output species amount contents, molalities, and activity coefficients.

MCS.rs4 – column output of calculated seawater state parameters (molality-based).

MCS.rs5 – column output of calculated seawater state parameters (amount content-based).

MCS_trace.res – this contains the fraction of each trace metal present in the solution that is free (uncomplexed), or complex by the inorganic anions present in the solution.

There are also three files with the extension .csv (for example, MCS.rs2.csv), which contain the same information as the files with normal column output but as comma separated values. These .csv files can be read directly into spreadsheet programs. (There is no .rs3 file.)

Other files (these should *not* be altered):

MCS.sen, Pitzer.mst, Pitzer.par, Pitzer.rcn

Subdirectory .\docs

_READ_ME_FIRST.txt – basic instructions concerning the download and how to get started.

List_of_files_trace_{version}.pdf – this file.

MCS_trace_manual_{version}.pdf – how to extract and run the model, and what the results mean.

MCS_alkalinity.pdf – how to adjust solutions for total alkalinity, total dissolved inorganic carbon, and total boron.

Notes

- There is no subdirectory ‘seawater’ or ‘ASWbuffer’ for this version of the model because there are no calculations of uncertainty.
- Successive runs of the model will overwrite the existing output files, so if you have results you want to save then move them to another directory.