



## List of files in this archive

### Top level directory:

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

#### Executable:

MCS\_sea.exe (Windows), or MCS\_sea (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).

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

### Subdirectories **.\\_iFix\_{1 – 11}**

Each of these eleven subdirectories contains the MCS.dat input file, and all results files, for a calculation for fixed seawater state parameter(s) for the eleven different problem types described in

the supplement to the manual. The example that is used, in all cases, is salinity 35 seawater at 25 °C.

## Subdirectory `.\docs`

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

`List_of_files_sea_{version}.pdf` – this file.

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

`MCS_sea_supplement_{version}.pdf` – how to run the model for cases where the input aqueous solutions are equilibrated to fixed, user-defined, values of seawater state parameters alkalinity, total dissolved inorganic carbon, pH, and  $p\text{CO}_2$  or  $f\text{CO}_2$ .

`MCS_alkalinity.pdf` – how to adjust solutions for total alkalinity, total dissolved inorganic carbon, and total boron. (This can now be done more easily using the methods described in the Supplement above.

## Subdirectory `.\seawater`

This contains a file `Uncert.mst` that should not be altered, and also a set of subdirectories (BC, CCA, AAC, NCA and `_lnKeql`) that contain variance information. The contents of these should also not be altered.

## Notes

- 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.