The MarChemSpec software package (see https://marchemspec.org) can be used to calculate chemical speciation in natural waters containing the ions present in seawater. MarChemSpec is not restricted to standard seawater composition, unlike CO2SYS and similar software. Thus carbonate equilibria, for example, can be calculated for natural waters with any major ion composition, and the same is true for the complexation of the trace metals that are the focus of GEOTRACES. The model results include estimated uncertainties.

Applications of MarChemSpec include not just the calculations of equilibrium concentrations, activities, and values of the four CO_2 seawater variables (pH_T, total alkalinity, total dissolved inorganic carbon, and pCO_2) but also saturation with respect to solid phases. Examples include various carbonate solids and alkalinity-enhancing minerals of interest in marine CO_2 reduction (mCDR) studies.

The chemical components included in MarChemSpec are:

• Seawater electrolyte (H^+, Na^+, Mg^{2+}, Ca^{2+}, K^+, Sr^{2+}, Cl^-, SO_4^{2-}/HSO_4^-, Br^-, F^-/HF, $B(OH)_3/B(OH)_4^-$, $CO_2/HCO_3^-/CO_3^{2-}$

• Trace metal cations Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Pb^{2+}, Al^{3+}, Fe^{3+}

Examples of the use of MarChemSpec in mineral dissolution and for calculations of trace metal speciation in seawater can be found in our Ocean Sciences 2024 posters (copies are on the MarChemSpec website, see the links in the August 2024 news item).

Software, and Information

For more information about the MarChemSpec project visit our website **https:\\marchemspec.org**. The software can be downloaded from there, where you will find the latest versions, or from our Zenodo archive **https://zenodo.org/records/8373046**.

Recordings of presentations explaining the use of the models are on YouTube **here**.

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If you have any questions, want to learn more about using the models, or want to become involved in new developments, please get in touch.

MarChemSpec was produced by SCOR Working Group 145, and since January 2023 its continued maintenance and development has been the responsibility of the Chemical Speciation Taskgroup of the IAPSO/SCOR/IAPWS Joint Committee on the Properties of Seawater.