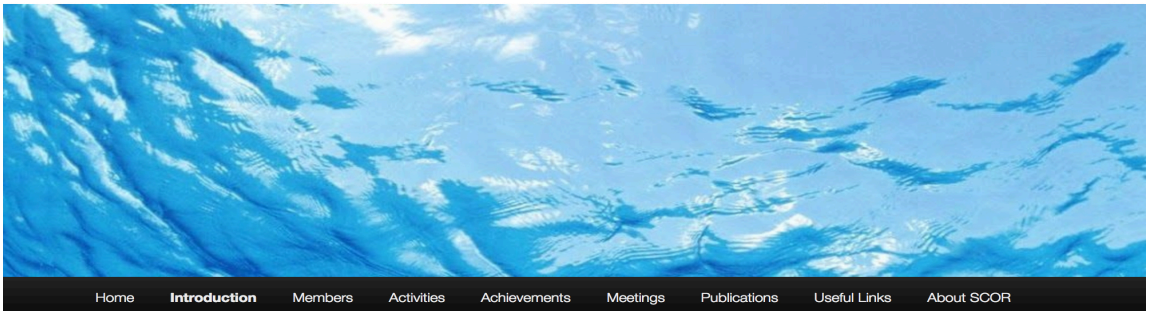
SCOR Working Group 145

MARCHEMSPEC: Chemical Speciation Modeling in Seawater to Meet 21st Century Needs



http://marchemspec.org

Rationale

The ability to model the biogeochemistry and especially the carbonate chemistry of the world's oceans, seas, and estuaries is required to understand and forecast environmental change due to human activity. However, the number of new studies yielding the activity, thermal, and volumetric data and stability constants needed to develop thermodynamic models, and extend our quantitative understanding of speciation in the oceans, has been in decline for many years. The numbers of skilled experimenters and modelers have also fallen. Furthermore, there is no comprehensive evaluation that relates the capabilities of speciation models, and the measurements they are based upon, to contemporary needs in chemical oceanography as exemplified in programs such as GEOTRACES.

Working Group Objectives

1. Document the current status, and basis in laboratory measurements, of Pitzer models of seawater and estuarine water and the complexation of key trace metals including Fe, Cu, Mn, Cd, Mn, and Zn. We will define current capabilities and limitations for oceanographic and biogeochemical calculations, and establish what is needed (in both laboratory measurements and modelling) to meet future requirements.

2. Provide a database of Pitzer model parameters and equilibrium constants for seawater (and their variation with temperature and pressure), including trace metal complexation, which can be used by skilled practitioners. The uncertainties, and the effects on calculated properties such as pH, will be evaluated.

Working Group Activities

1. **Town Hall Meeting at 2016 Ocean Sciences Meeting:** *Toward a Standard, User-Friendly Chemical Speciation Model for Seawater and Estuarine Waters* to engage with and query the chemical oceanography community on key priorities, interests and needs associated with a new chemical speciation model for community use.

2. **Community surveys:** Following up on feedback received at Town Hall Meeting, WG members developed and broadly distributed web surveys to various potential user groups (total of 166 responses) on specific aspects of the speciation model (e.g., platform, user interface, training tools, etc.); results are being prepared for publication and dissemination, and will guide the development of user-friendly software for chemical speciation modeling.

3. **Article in *Frontiers in Marine Science*:** WG members published an article entitled '*Towards a quality-controlled and accessible Pitzer model for seawater and related systems*' (Turner et al., 2016 *Front. Mar. Sci.* **3**, 139, https://doi.org/10.3389/fmars.2016.00139).

4. **Funded project:** Our 3 year project "*A Thermodynamic Chemical Speciation Model for the Oceans, Seas, and Estuaries*" (funded by NERC/NSF) began in November 2017. Laboratory measurements (predominantly Harned Cell measurements) will be carried out at Scripps Inst. Oceanography (A. Dickson), and model development at Univ. East Anglia (S. Clegg). Heather Benway (Woods Hole Oceanographic Inst.) is responsible for links to our user community.

   Collaborations with the national metrological institutes of Germany (**PTB**), France (**LNE**), and Japan (**NMIJ**) (all of whom who will carry out experiments) have enabled us to focus initially on a chemical speciation model of the Tris/TrisH$^+$ buffers used to define the marine pH scale and to calibrate pH instrumentation, with particular emphasis on the 'traceability' of the model and the propagation of measurement errors. Other contributors of new measurements are **GEOMAR** in Kiel, and potentially a group at the **Univ. of Belgrade**. The Working Group is collaborating with researchers at **NIST** in the USA, and the **Universities of Delaware** and **South Florida**, who are carrying out related work on marine pH.

For More Information

We welcome the interest and input of marine scientists. Please contact the Chair **David Turner** (david.turner@marine.gu.se) for information about the Working Group activities; and either **Simon Clegg** (s.clegg@uea.ac.uk) or **Heather Benway** (hbenway@whoi.edu) regarding the funded project described above.