

To: Joint Committee on the Properties of Seawater (JCS)
International Association for the Physical Sciences of the Oceans (IAPSO)
International Association for the Properties of Water and Steam (IAPWS)
Scientific Committee on Ocean Research (SCOR)

From: SCOR Working Group 145 “MarChemSpec”

We propose that JCS create a new Taskgroup to continue the work of SCOR Working Group 145

Background

The vision that guides our work is “*The marine science community will have free access to fully documented, state of the art, user-friendly software for chemical speciation calculations, including uncertainty estimates*”. A first version of this software will be released in the autumn of 2022, following which SCOR Working Group 145 will be disbanded having fulfilled its terms of reference. This is in accordance with normal SCOR practice since all Working Groups have a limited lifetime.

Our work is, however, far from complete. Documentation and testing of the chemical speciation models that lie behind the 2022 software release have allowed us to identify shortcomings and to prioritise the work needed for model improvement. For this continuing work, which includes an active experimental programme, there is much to be gained from a formal association with a respected international organisation. This would both give the software products international visibility and recognition and help to attract the support of new collaborators and of funding agencies.

More information is available at the website marchemspec.org.

Why JCS?

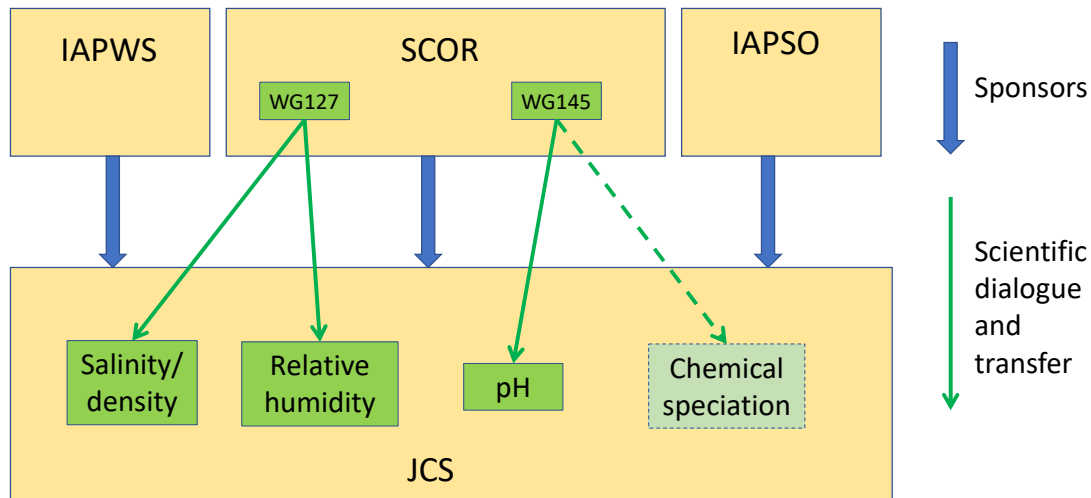
The Joint Committee on the Properties of Seawater arose from SCOR Working Group 127, which established the absolute salinity scale and derived a Gibbs function for calculation of the bulk physical properties of seawater. JCS is now meant to provide a permanent, continuous, ongoing “home” for expertise in these areas. In turn, we believe there is a need for a permanent, continuous, ongoing “home” for expertise in the chemical properties of seawater. In addition, the need to work with standards-development organizations like IAPWS as well as oceanographic organizations like SCOR and IAPSO, and perhaps (in future) with chemistry organizations like IUPAC is very similar to current JCS practices.

Why a new Taskgroup?

JCS has an established Taskgroup on seawater pH, that has largely been concerned with work towards SI traceability. The work of SCOR WG145 on the modelling of Tris buffer chemistry has contributed significantly to this Taskgroup. However, the proposed speciation Taskgroup has both a broader focus (to support other chemistry issues, e.g., including trace metals, with speciation calculations) and one that is not as technically focussed on pH itself. A different (albeit slightly overlapping) set of scientific experts are involved.

The relationships between these two SCOR Working Groups and the JCS Taskgroups, including the proposed chemical speciation Taskgroup, are shown in the diagram below. Given the existing links between SCOR WG145 and JCS, the proposed new Taskgroup is a logical development.

Relationships between SCOR Working Groups and JCS Taskgroups



Benefits for JCS

The proposed new Taskgroup on chemical speciation would broaden the remit of JCS from a largely physical focus to include a substantial chemical component. This would complement the work of the pH Taskgroup, make the work of JCS relevant to a larger community of marine scientists, and thus benefit both JCS and its two marine sponsoring organisations (SCOR and IAPSO).

Terms of Reference

The proposed new Taskgroup could be given Terms of Reference similar to those for JCS. Alternatively, the JCS Terms of Reference could be expanded by replacing references to TEOS-10 with TEOS-10 and chemical speciation; and referring to bulk physical properties and chemical speciation in seawater.

Proposed Taskgroup membership

The majority of the proposed membership are Full or Associate members of SCOR Working Group 145, ensuring continuity through the transition to JCS. The combination of senior and mid-career researchers provides the basis for succession planning: this is an important consideration since the model development in SCOR Working Group 145 has been largely driven by senior researchers. In terms of expertise there is a strong focus on trace metals and their interactions with natural organic matter, which is a major priority for the future. This group will maintain close contact with the Taskgroup on pH, which includes several members of SCOR Working Group 145 (Simon Clegg, Frank Bastkowski, Andrew Dickson, and Daniela Stoica). The following researchers are proposed as Taskgroup members:

- Bob Byrne, University of South Florida, USA, rhbyrne@usf.edu
- Simon Clegg, University of East Anglia, UK, s.clegg@uea.ac.uk
- Peter Croot, NUI Galway, Ireland, peter.croot@nuigalway.ie
- Martha Gledhill, GEOMAR, Germany, mgledhill@geomar.de
- Pablo Lodeiro, University of Lleida, Spain, pablo.lodeiro@udl.cat
- Sylvia Sander, GEOMAR, Germany, ssander@geomar.de
- David Turner, University of Gothenburg, david.turner@marine.gu.se (chair)

Financial implications

During the last two years we have worked efficiently without physical meetings. Regular fortnightly meetings of an active core group have been complemented with smaller ad hoc meetings and larger annual meetings, all online. Funding for physical meetings is thus not a priority, although members will of course take advantage of participation in scientific meetings funded from other sources.

We will continue to seek research funding to support the planned developments described in the Appendix.

There is one Taskgroup cost that is unavoidable: the website that will host the software and related information. This has yet to be built. There is funding for this, but from January 2023 onwards support may be required for ongoing costs of hosting and maintenance.

Appendix: Current status and future priorities

Over the last few years, our work has focused on three areas:

- Documentation of existing chemical speciation models
- Software development
- New experimental measurements relevant to the modelling of Tris buffers in artificial seawater, contributing to the JCS Taskgroup on pH.

A key source of funding for the documentation and software development has been the joint NERC/NSF project *A Thermodynamic Chemical Speciation Model for the Oceans, Seas, and Estuaries* awarded to three SCOR WG145 members (Benway, Clegg, and Dickson). The documentation of the chemical speciation models has included review of all the original thermodynamic measurements that contribute to the model together with comparisons with published measurements in multicomponent systems. This work is being prepared for publication in four papers. The first two papers, on artificial seawater and on Tris buffers, are in press in the journal *Marine Chemistry*. Documentation for the third paper on the seawater electrolyte (Na, Mg, Ca, K, Sr, Cl, SO₄, CO₃, B, Br, F) is complete: documentation for the fourth paper on the GEOTRACES core elements is under way.

The new experimental measurements have been carried out at GEOMAR (Germany) and the national metrological institutes in France, Germany, Japan, and the United States within the overall SCOR WG145 programme. The work at GEOMAR on Tris solubility has been published in the *Journal of Chemical and Engineering Data*. The programme of work at the national metrology institutes is nearing completion.

Future priorities include improvement and extension of the modelling software and its applications:

- Analysis and integration of existing thermodynamic datasets in the literature to ensure that all coefficients in the model lie within a consistent framework: the documentation of existing models has revealed shortcomings in this respect.
- Extension of the model to include additional trace elements and interactions with natural organic matter
- New thermodynamic measurements of key interactions that have not been studied in sufficient detail.
- Collaboration with relevant research groups to develop applications for the software in different areas of aquatic geochemistry.