

1. Introduction

This first meeting of the group focused on planning. Issues discussed included: the seawater components and trace elements, and ranges of physicochemical conditions, to be covered (based upon user needs); the allocation of tasks; compilation of a list of external contacts for consultation; and plans for securing additional funding. The results of the meeting, for each of these areas, are described below.

2. Scope of the planned review of marine speciation modelling

The first task for this WG is to define the scope of the review of available models and data for the calculation of speciation in seawater, in terms of both environmental conditions and chemical components. This work contributes to Objectives 1 and 2 in the WG Proposal. A draft was generated on the afternoon of 12 April, and reviewed on 13 April. It was agreed that each item in the planned scope would be accompanied by a short justification explaining which global questions and/or problems can be addressed by modelling particular ions and trace species, and the environments in which they are important. These texts will form an essential component of the various activities aimed at maximising the visibility of the WG (see § 4 below), and will also help justify new work to fill gaps in the availability of the necessary thermodynamic information.

The Tables below give the allocation of responsibilities, and the priorities of the different chemical systems and environments. They include buffers and ligands used in the laboratory for titration and for calibration. The texts are expected to be complete, and collated, by mid June 2015.

Table 1: Environmental Conditions		
Priority		Writer
1	Oceans	-
1	Temperature -2 to 40°C	-
1	Pressure up to 1100 atm	-
1	Estuaries (including groundwater discharges and river end members)	Arthur Chen
2	Polar brines, temperatures below 2°C	Eric Achterberg
2	Pore waters	Vanessa Hatje
2	Sulphidic conditions	Maite Maldonado
2	Temperature up to 100°C for diffuse hydrothermal discharges	Sylvia Sander
3	Inorganic contaminant inputs	Eric Achterberg
3	Temperature up to 300°C for mixing of hot hydrothermal discharges	Sylvia Sander
4	Salt lakes and brines	Simon Clegg

Table 2. Major and minor components		
Priority		Writer
1	Major ions of seawater (Na ⁺ , Mg ²⁺ , Ca ²⁺ , K ⁺ , Cl ⁻ , SO ₄ ²⁻), pH (H ⁺), carbonate species (CO ₂ , CO ₂ [*] , HCO ₃ ⁻ , CO ₃ ²⁻)	-
1	Weak acids and bases: bisulphate, borate, fluoride, phosphate, ammonia	David Turner
2	Silicic acid	David Turner

Table 3. Trace metals (* = redox active)

Priority		Writer
1	Fe*, Cu*, Zn, Cd	David Turner
2	Mn*, Co, Ni,	David Turner
2	Pb, Hg (and MeHg)	Mona Wells
3	Cr*, As*, Ag, Al, Ln(*)	Mona Wells

Table 4. Buffers and indicators (laboratory conditions only)

Priority		Writer
1	pH buffers: tris, aminopyridine	David Turner
1	CLE-CSV buffers: EPPS, HEPES	Stan van den Berg
1	Indicators: m-cresol purple, thymol blue, bromocresol green	David Turner

Table 5. Complexants* (laboratory conditions only)

Priority		Writer
1	CLE-CSV competing ligands: SA, NN, APDC, DHN	Stan van den Berg
1	”Standard” ligands: EDTA, DTPA, DFB	Sylvia Sander
1	S ligands: glutathione, cysteine, thiourea	Sylvia Sander
2	Cyclam, cyclen	Maite Maldonado
3	”Standard” ligands: NTA, DFE, more siderophores	Maite Maldonado
3	CLE-CSV competing ligands: DMG, TAC	Sylvia Sander

* Humic materials have also been discussed as Complexants. These will not be included in the Pitzer model, but coded separately e.g. according to the WHAM or NICA-Donnan formulations.

3. Planning the review of existing seawater, and seawater-related, Pitzer models

This was a subgroup meeting held on the afternoon of 13 April. The participants were Simon Clegg, Darren Rowland, David Turner and Mona Wells. It was agreed that the first priority would be the major, minor and trace components of seawater. The following order of actions was agreed:

- **Simon Clegg** will document the data sources used by the Miami (Millero) and Clegg & Whitfield models for major and minor species of seawater (first and second rows of Table 2 above)
- **David Turner** will document the data sources used by the Miami model for trace elements (Table 3 above)
- This documentation will be passed to **Darren Rowland**, who will check whether the JESS database contains later information that is relevant to the interactions and model parameters

that have been documented. Some literature searches independent of JESS will also be carried out.

- The results will form the basis of a review of data and parameter availability calculations of speciation involving the relevant ions and trace elements in seawater. Our initial results and work-in-progress will be presented at the planned 2016 Town Hall meeting, and submitted for publication during early 2017. Potential journals were discussed, including marine chemistry journals, *ES&T*, and *Environment International*.
- The data review for buffers, indicators and ligands will be carried out and published separately to the review of the major and minor species. It was generally recognised that, given the size of the project, publication in two or more parts would be appropriate.

4. Activities to maximise the visibility of WG145 activities in the marine science and chemical communities

Based on experience from previous SCOR WGs, Arthur Chen and Sylvia Sander emphasised the need to act on this point as soon as possible so as to ensure the that final product is well known and thus has a good chance of being accepted and used by the marine science community. Using the speciation model scope as the basis of this initial dissemination will allow interested scientists to comment on this scope, and contribute to it, and thus ensure a broad acceptance.

- An article presenting the WG and scope in *EOS* (**David Turner** to make contact and coordinate writing)
- An article presenting the WG and scope in *Chemistry International* (**David Turner** to make contact and coordinate writing)
- An article presenting the WG and scope in *Elements* (**Sylvia Sander** to make contact and coordinate writing)
- An article presenting the WG and scope in *Frontiers in Marine Biogeochemistry*, in the WG139 special issue (Editor **Eric Achterberg**; **David Turner** to coordinate writing)
- A WG website, to be hosted at Otago University, following a similar structure to the WG139 website (responsibility: **Sylvia Sander**)
- A Special Session on speciation modelling at Ocean Sciences 2016 (application deadline 29 April, responsibility: **David Turner** and **Sylvia Sander**)
- A Town Hall meeting at Ocean Sciences 2016 (applications open in July, responsibility: **David Turner** and **Sylvia Sander**)
- Establishment of a mailing list of interested scientists. **Sylvia Sander** will ask scientists on the WG139 mailing list if they also wish to be on the WG145 mailing list.

The articles listed above should be submitted, and preferably published, before the end of 2015.

5. External funding opportunities

Additional funding for both senior scientist and postdoc time would be valuable in developing the Pitzer database for marine applications. Further funding will also be essential for developing the user-friendly web-based calculation program described in the terms of reference. Based on the WG discussion, **Simon Clegg** will compile a list of potential funding opportunities, identifying the individual WG members responsible for investigating each opportunity in further detail.

6. Additional expertise

The need for additional expertise, complementing the WG membership, was discussed. A shortlist of names was identified. The WG Chair and Vice-chairs will sound out these individuals' interest in attending the 2016 meeting as guests, and contributing to WG activities.

6. Review of existing (non-Pitzer) speciation modelling programs

A task for the WG is to develop specifications for a web-based speciation modelling tool (Objectives 3 and 4 of the Proposal). As a first step, the WG members will review the user interfaces of some existing programmes in order to identify capabilities that are appreciated by users. More than 10 programs (that members already have experience of) were identified. It was agreed that these would first be reviewed by WG members experienced in their use. **Simon Clegg** will compile the list of programmes with a nominated reviewer for each programme, and a questionnaire to be completed by the reviewers.

7. Plan for the next meeting

The next meeting will be held in conjunction with the 2016 Ocean Sciences Meeting in New Orleans, USA. The provisional date is 21 February, the day before the Ocean Sciences Meeting opens. The following agenda items will be covered:

- Adjustments to the modelling scope, following comments received
- Status of the data availability review
- External funding opportunities
- Workshop on the user interface of existing modelling programmes

8. Thanks to the local host

The WG expressed their sincere appreciation to Ivanka Pižeta for her tireless and efficient support.

Appendix 1. Meeting programme

12 April

9:00	Introduction: background to the WG and project plan	David Turner
9:30	WG members present themselves (1-2 minutes each)	
9:45	Project scope: Summary of questionnaire replies and draft project scope	Sylvia Sander
10:30	Coffee	
11:00	Talk: overview of chemical speciation modelling	Simon Clegg
11:45	Talk: modelling natural organic matter chemistry	David Turner
12:30	Lunch	
13:30	Talk: The TEOS standard for seawater	Arthur Chen
14:15	Discussion: scope of the project	
15:00	Coffee	
15:30	Discussion: scope of the project	
17:30	End of Day 1	

13 April

9:00	Scope of the project: discussion of the revised draft
10:30	Coffee
11:00	Discussion: additional contacts and potential external funding (questions 9 and 10 in the questionnaire)
11:45	Assignment of tasks in preparation for Meeting no. 2
12:15	Next meeting: time, place and meeting plan
12:30	Lunch

Afternoon session for speciation modellers only:

13:30	Discussion on the scope of the review paper (Deliverable 1 of the WG)
14:00	Discussion on the work to be done to meet Objectives 1 and 2. This includes collection and review of relevant physico-chemical information for the seawater electrolyte; analyses of current Pitzer parameter databases for data sources and coverage of agreed systems and environmental conditions; uncertainty analysis.
15:00	Coffee
15:30	Discussion continues
16:30	Discussion on potential external funding for the above and later work of the WG.
17:00	Assignment of tasks.
17:30	Meeting ends

Appendix 2. Participants

David Turner, chair

Simon Clegg, vice-chair

Sylvia Sander, vice-chair

Eric Achterberg

Arthur Chen

Vanessa Hatje

Maite Maldonado

Ivanka Pižeta

Darren Rowland

Rodrigo Torres

Stan van den Berg

Christoph Völker (12 April only)

Mona Wells