Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS)

Report to SCOR and IAPSO on JCS Workshops Sept 2018

and

Recommendations on renewal of Terms of Reference and membership

Executive Summary: JCS reports on activities over the last 5 years, including relevant publications by their members (Appendix C). As a result of discussions at a recent set of workshops, convened 5 years after an initial set of workshops that formulated the basic goals of JCS, our recommendation to SCOR, IAPSO, and IAPWS is that:

a) JCS continue as an organization sponsored by SCOR, IAPSO, and IAPWS,

b) that the JCS Terms of reference (Appendix A) remain unchanged for the next cycle, and

c) that the membership of the various JCS taskgroups (Appendix B), which are largely independent of one another, be increased slightly to assist them in their work, by including a number of scientists who are currently contributing to the tasks of JCS.

JCS Activities (2013-2018)

JCS was formed in 2012/2013 when terms of reference and a proposed executive (chairman and two vice-chairs) were approved by all parent organizations (SCOR, the Scientific Committee on Oceanic Research, IAPSO, the International Association for the Physical Sciences of the Oceans, and IAPWS, the International Association for the Properties of Water and Steam). Following this approval a more extensive membership was developed, and JCS subsequently met as group in Sept. 2013, when a series of workshops were held in conjunction with the 16th International Conference on the Properties of Water and Steam (ICPWS16, Greenwich, UK). At this meeting taskgroups were formed for "salinity/density", "pH", and "Relative Humidity (RH)", and a separate workshop held for each. The outcome of these workshops was a set of goals and activities. JCS has not meet formally as a group in subsequent years, although informal meetings of JCS members have occurred throughout this time, often during IAPWS annual meetings.

During 2013-2018, JCS activities can be separated into 3 categories:

Ongoing support for TEOS-10, which included:

- Maintenance of the TEOS-10 web site (www.teos-10.org), including the development of

pedagogical material (slides, lecture notes) to be distributed there.

- Maintenance and expansion of the extensive TEOS-10 software suite.
- Providing advice on the incorporation of TEOS-10 equations and software into oceanographic numerical models (now in NEMO, MOM6, MITgcm, and ROMS), as well as into CTD vendor software (now in Seabird and RBR software suites).
- Maintenance of the TEOS-10 Manual (minor corrections and updates).
- Replies to external questions (generally email) about TEOS-10 issues.
- Reporting on JCS activities to parent organizations.
- Writing of support letters for TEOS-10/JCS-related research proposals when requested.
- Reviewing journal articles on TEOS-10 topics.
- Providing a forum and a community for the exchange of information on laboratory, field, and theoretical developments related to TEOS-10.
- Encouraging technical collaborations between JCS members (and others).
- Providing a focus for TEOS-10-related work as part of the IAPWS Annual Meetings (which have been generally attended by a small fraction of JCS members as interests and outside funding permitted; SCOR has generally provided travel support for 1 or 2 JCS members to attend this meeting each year)

Research Activities, (mostly resulting or aimed to result in publications, see list in Appendix C) which include:

- Carrying out the technical tasks agreed on at the 2013 Workshops
- Encouraging the acquisition of more field data on "Salinity anomaly" δS_A (roughly tripling the number of oceanic data points);
- Encouraging published intercomparisons between OSIL-provided IAPSO Standard Seawater and a Chinese SSW product that is made independently.
- Encouraging new (metrological) measurements of the absolute density of seawater.
- Encouraging the development of techniques to provide high-quality relative density measurements using Vibrating-Tube Densimeters.

Providing Information to the Oceanographic and Metrological Communities

- In addition to the extensive list of publications related to JCS tasks (see Appendix C), a series of 4 comprehensive overview papers were published in the journal Metrologia in 2016 outlining the issues surrounding the present state of practice in the 3 taskgroup areas, as well as future plans (Feistel et al., 2016, Pawlowicz et al., 2016, Dickson et al., 2016, Lovell-Smith et al., 2016)
- JCS formed links with SCOR WG-145 (Speciation of Seawater) to suggest modification

to their work plan that might assist in the goals of JCS.

- Oceanographers in JCS have attended the invitation-only meetings of the Electrochemical and Humidity Working groups (BIPM/CCQM-EAWG and BIPM/CCT-WG-Hu) at the International Bureau of Weights and Measures (BIPM) to lay the groundwork for future developments towards making seawater properties "traceable to the SI" (travel funding provided by IAPWS)
- JCS members have provided advice at IOC activities (e.g., RF attended the 4th JCOMM Marine Instrument Workshop for ASIA-PACIFIC, Weihai, China, 21-23 Oct. 2014 as a JCS representative, at the invitation of the GOOS Project Office (IOC/UNESCO)).

JCS: 2018 Workshops

Under the conditions of its formation, the terms of reference for JCS must be approved every 6 years. A proposal was put forward to SCOR and IAPSO to have JCS meet formally as a group for a 2nd time at a similar series of workshops to be held at the 17th International Conference on the Properties of Water and Steam (ICPWS17, Sept/2018, Prague, Czech Republic). Some travel support was provided by both SCOR and IAPSO. Separate workshops were held for each of the 3 taskgroups, with a fourth workshop to revisit the overall structure, aims, and terms of reference of JCS itself. 12 JCS members attended, missing were Vice Chair RF (health issues), Industry representatives BL and RW, and salinity/density taskgroup members FM and YP.

1. JCS Workshop (14 attendees): This workshop began with an overview by RP (JCS Chair), and a historical perspective from an oceanography point of view by TM (JCS Vice Chair). Issues discussed were:

JCS Terms of Reference: It was decided that the terms of reference (Appendix A) should remain unchanged.

Executive: TM will be replaced by SS as Vice-Chair (approved by workshop participants). Retention of RP as Chair and RF as Vice-Chair was also approved.

Membership: Although the general membership structure still seemed suitable, it was generally felt that the membership of individual taskgroups needed to be increased. Each taskgroup has a membership that is independent of that from other taskgroups, but is generally working as a group with other not-currently-JCS scientists who would benefit from formal membership. The proposed membership is fully listed in Appendix B. Changes approved by JCS at this meeting are:

- Salinity/density Taskgroup: Addition of Yohei Kayukawa (AIST, Japan) and Ryan Woosley (MIT, USA). YK collaborates with HU and is carrying out absolute density measurements of seawater. RW has recently left FM's laboratory, but is carrying out collaborations with RP and HU on field measurements of salinity anomaly, and has volunteered to coordinate the best practises document.

- pH Taskgroup: Addition of Frank Bastkowski (PTB, Germany) and Simon Clegg (UEA, UK). FB has primary responsibility for pH measurements at PTB, and SC is Vice-chair of SCOR WG145, working with AD and other members of the pH taskgroup on the development of a traceable Pitzer model.
- RH Taskgroup: Addition of Stephanie Bell (NPL, UK) to RH taskgroup. SB is chair of BIPM-CCT-Wg-Hu and is providing strong support to the effort to define RH.

In addition, we are now designating "Taskgroup Chairs" to lead the taskgroups. These are Pawlowicz (salinity/density), Dickson (pH), and Lovell-Smith (RH).

Software: Current software is now available on github and would-be developers can apply to PB for editing access if they wish. TM also reports that CSIRO (AUS) is funding some translations of the software into additional computer languages. Software is also being written by the RH taskgroup and all agree that the TEOS-10 website would be a good place from which this can be served; PB can provide advice to facilitate this.

Web Services: TM/PB are exploring a transition of the website to be served by TM's home university (UNWS, AUS) which should allow it to exist into the foreseeable future.

Updates to TEOS-10: At this point there is not enough data and/or pressing need to update PSS-78, TEOS-10, or the TEOS-10 Salinity Anomaly database. However, it was agreed that a white paper for the web site should be written (led by RP) outlining the known problems with TEOS-10 and issues to be resolved in future, to make this information more generally known.

Publications – a new "special issue"?: It was felt that there were not enough publications currently planned to make a useful special issue; instead the strategy of continuing to publish papers singly in different journals would be more important to maintain awareness of JCS issues. Also, it was suggested that the IUGG meeting (Montreal, July/2019) would be a suitable venue for presentations on JCS issues and JCS members are encouraged to submit an abstract there.

2. Salinity/Density Workshop (19 attendees). This workshop began with an overview of progress towards traceability by SS, and an overview of attempts to determine absolute density by YK. A variety of issues were then discussed:

SSW Conductivity: The current consensus is that after further work, traceability to the SI of absolute conductivity at the level required is still not possible. However, more measurements of conductance at high temperatures, pressures, and salinities would be useful and plans are underway to carry out these measurements (SS).

Absolute density Measurements: are currently being attempted by YK and A. Albo (INRiM, Italy). However, many issues (some related to sample handling) are yet to be resolved.

Relative Density Measurements: Over the last few years different groups have been reporting contradictory results about whether Anton Paar densimeters are measuring the density of OSIL SSW to be a) in accord with TEOS-10, or b) lower by 5-15ppm lower than TEOS-10. Resolving this problem is critical, and there are two actions that can be taken:

1. Develop a "best practices" guide that compares and contrasts the methodology of all groups performing these measurements (HU, SS, SW, coordinated by RW)

2. Collate all available information about the chemical characteristics of SSW (batch-to-batch variations in density, density anomaly, conductivity, nutrient levels (RW, SS, SW, coordinated by HU).

SSW: Keeping track of the composition of SSW will clearly be important into the future. Currently this is being carried out in an ad-hoc way; it is suggested that a more reliable procedure would involved suggesting to IAPSO at some point in the near future that this becomes a formal part of SSW manufacture.

3. pH Workshop (17 attendees). The workshop began with an overview of recent progress by AD, presenting slides by FB who was absent for health issues, and an overview of the plans and progress of SCOR WG-145 (Chemical speciation modelling in Seawater) by invited speaker S. Clegg. The current focus of their work, with an expanded group of collaborators including pH taskgroup members DS and FB, is in understanding fully how pH_T is determined using spectrophotometric measurements with m-cresol purple (including their link to measurements using primary Harned cells). A key part of this is the development of a traceable Pitzer speciation model of pH_T in Tris buffers in artificial seawater. This was suggested as task #4 in the Metrologia paper of Dickson et al. (2016).

The general plan as outlined in the Metrologia paper (Dickson et al., 2016) was accepted as the basis for future work and will continue to be implemented, with these immediate goals:

Uncertainty Budget for pH_T measurements: A draft formal description of exactly how the measurement of pH_T is performed and calibrated (using techniques similar to those of PTB and IoW in their recent papers in Frontiers of Marine Research will be prepared (led by AD, circulated to pH Taskgroup and other interested parties). Once the text is agreed, this would then be used in discussions with BIP-CCQM Working Group on Electrochemical Analysis (CCQM-EAWG, SS and DS are members) and with the IUPAC Subcommittee on pH (FC is chair, DS, FB, AD are members) for additional comment, and for help in preparing a well-founded uncertainty budget for the measurement of pH_T in seawater media, and a clear statement of its traceability chain.

Links between spectrophotometric and glass electrode methods: Glass electrode measurements calibrated using low-ionic-strength buffers are typically used in water quality measurements, but spectrophotometric methods based on TRIS are used in the ocean. AD will provide DS with a simple procedure to link pH (measured using glass electrodes) to an approximate value of pH_T for seawater which she will test in her laboratory, and they will try to develop a convenient and meaningful quality control protocol for such measurements.

Future of the Pitzer model: SCOR WG-145 expects that the traceable Pitzer model of pH_T will be expanded in the future to include carbonate and borate equilibria in seawater and to be developed into a publically available set of modelling tools.

4. RH Workshop (16 attendees). The workshop began with an overview by OH on the current state of

understanding and knowledge, followed by JLS & RF on the progress in developing a generalised metrics of relative humidity, and finally by SB on the RH definition and how it fits with SI (International System of Units) metrology and NMI (National Metrological Institutions) practices in realisation of humidity standards. The following discussion concerned:

Basic challenge: Generalisation of the RH definition is a superposition of three tasks: (a) the scientific understanding of relevant thermodynamic theory, (b) a metrological task aimed at an adequate technical realisation of RH, and (c) a communication-interaction process between theoreticians, metrologists, and practitioners.

Communication aspects: There is a general need for a common language to effectively communicate the aims of the JCS RH taskgroup and the theoretical background of the new metrics through and within a broader community of hygrometrologists and practitioners. SB proposed to guide the further discussion along the following big five (RC-TEC): R = relevance, C = clarity, T = transparency, E = equivalence , C = consensus (details will be outlined in the Technical Report of the workshop). Towards that end:

1. The JCS RH taskgroup should continue to exist and continue with its activities.
2. Software (for fugacity and relative fugacity, mutual transformations between humidity measurands, sensitivity and uncertainty analysis) should be distributed on the TEOS-10 web site (with TEOS-10 software) to make it more widely available.
3. A non-mathematical communication paper guided by the RC-TEC challenges should be prepared, to be published in a meteorological (not metrological) journal.

An agreed-on definition? The discussion revealed that there is no essential scientific disagreement among the involved participants, but the current state of mutual understanding of the scientific, metrological, and user-specific aspects does not yet allow us to formulate an "agreed" position on a generalised RH definition. Different definitions each have their own advantages and disadvantages, which are often relevant to particular sectors of the community. There was technical discussion about the “fundamental” nature of mole-based vs. fugacity-based definitions. To continue, the taskgroup should

1. Prepare a paper to clearly communicate to the educated non-specialist the basics of RH, enhancement factor, etc.

Initial reactions: A central subject of the discussion were the implications resulting from communications between IAPWS president Prof. Kretzschmar (Germany), IAMAS president Prof. Turner (Cambridge), IAPSO vice-president Prof. McDougall (Australia), and International Commission on Clouds and Precipitation (ICCP) vice-president Prof. McFarquhar (U.S.) regarding a possible cooperation and propositions on the problem of a generalised humidity definition. A generalisation of the RH metrics is, for traceable reasons, not currently on the ICCP agenda. Further cooperation with ICCP is considered indispensable for better communication across the involved disciplines, and, in fact, it appeared that the most work in future must be devoted to the communication-interaction task. SB emphasised, e.g., the need for a perception of a generalised RH metrics throughout the whole hierarchy of the metrological community. The realisation of the RC-TEC requirements is considered a basic requirement for placing the problem of a generalised RH definition on the BIPM agenda. The following tasks will be carried out:

1. Prepare a thoughtful response to concerns expressed by ICCP.

2. OH plans to give a talk at the 27th IUGG General Assembly in July 2019 in Montreal on the statistical significance between the standard and generalised RH metrics, emphasizing that the generalisation of the RH definition is neither primarily intended for nor restricted to meteorological applications, but covers all subcritical regions of the p-T phase diagram of water.

OH summarized: Every problem listed on the agenda can be solved. However, now we have identified the problem, but we are still not clear on what the solution will look like – although getting there will require discussion in the larger community.

R. Pawlowicz

JCS chair, Oct 11 2018

Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS)

Appendix A: JCS Terms of Reference

The purpose of the Joint SCOR/IAPSO/IAPWS Committee on the Properties of Seawater is:

1. To act as a 'point of contact' for issues related to the bulk properties of seawater.
2. To maintain and update documents, websites and software of TEOS-10 and other standards.
3. To encourage the uptake of TEOS-10 and other standards by the oceanographic community by acting as a source of advice.
4. To globally coordinate research and the development of standards related to properties of seawater across different scientific communities.
5. To identify developing needs for standards and encourage research in those areas, through small collaborations, more formal Working Groups, conference sessions, or other avenues.
6. To issue reports or other documents from time to time on issues relating to the bulk properties of seawater.
7. To work toward international and interdisciplinary uniformity and consistency of the standards and measurement procedures used in oceanography

Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS)

Appendix B: Membership

Membership

Executive	
Rich Pawlowicz (Chair)	Canada
Rainer Feistel (Vice-chair)	Germany
Steffen Seitz (Vice-chair)	Germany
Salinity/Density Taskgroup	
(Rich Pawlowicz) (Chair)	
Frank J. Millero	USA
(Steffen Seitz)	
Hiroshi Uchida	Japan
Stefan Weinreben	Germany
Youngchao Pang	China
Ryan Woosley	USA
Yohei Kayukawa	Japan
pH Taskgroup	
Andrew Dickson (Chair)	USA
Maria Filomena Camoes	Portugal
Daniela Stoica	France
Simon Clegg	UK
Frank Bastkowski	Germany
Relative Humidity Taskgroup	
Olaf Hellmuth	Germany
Jeremy Lovell-Smith	New Zealand
(Rainer Feistel)	
Stephanie Bell	UK
Export subgroup: Thermodynamics	
(Rainer Feistel)	
Expert subgroup: Numerical Modelling and Applications	
Trevor J. McDougall	Australia
Expert subgroup: Software	
Paul Barker	Australia
Industry Representatives	
Richard Williams (OSIL)	UK
Barbara Laky (Anton Paar)	Austria

Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS)

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Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS)

Appendix C: Papers and other material published on JCS topics by JCS members (2013-2018)

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11. Feistel, R., Lovell-Smith, J.W., Hellmuth, O. , Virial Equation for the Fugacity of Water in Humid Air. International Journal of Thermophysics 36, Issue 1, pp. 44-68 (2015).
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Fugacity of H2O in Humid Air.The International Association for the Properties of Water and Steam.Stockholm, Sweden, July 2015

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