SCOR/IAPSO WG 127 on the Thermodynamics and Equation of State of Seawater Updated Progress Report to SCOR, September 2008

Full Members

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1. Working Group Meetings

SCOR/IAPSO WG127 was approved in 2005, had its first meeting at Warnemünde in May 2006, its second meeting at Reggio, Italy in May 2007, and its third meeting on 3-9 September 2008 in Berlin. The second and third meetings in May 2007 and September 2008 were attended by all full members except Valentina Gramm-Osipova.

2. Requests to SCOR concerning membership or terms of reference

None at this time.

3. Activities between working group meetings

Many of the issues on our agenda are being pursued by individual members, and by subcommittees of WG127, and we expect substantial progress on many issues between meetings of the Working Group.

4. Next Working Group Meeting

The third meeting of the working group has just recently occurred from 3-9 September 2008 in Berlin. This meeting consisted of four days of exclusively WG127 meeting, followed by a day (a Sunday) during which members of WG127 were observers at the executive meeting of IAPWS (the International Association of the Properties of Water and Steam). During this Sunday meeting we saw IAPWS officially bless our saline Gibbs function, and release it as the Release IAPWS-08. On the following day Trevor McDougall gave a keynote address about the work of WG127 and we also met with Dr Keith Alverson, executive director of IOC. The next day (Tuesday 9th September) most members of WG127 presented scientific talks at the IAPWS symposium in Berlin.

At our Working Group meeting in Berlin we made progress on many issues including that of constructing a suitable algorithm for calculating Absolute Salinity. Given the time required to complete this work and the work that still needs to be done to finalize all the other computer software, it became obvious that we would not be in a position to have IOC adopt our work by mid 2009; rather an extra year will be required.

5. Assessment of Progress

As of September 2008, WG127 has reached the point of having finalized the new definition of salinity (Absolute Salinity, publication #11 below), and of the saline Gibbs function (publications #2 and #7 below). When added to the existing official thermodynamic definitions of pure water substance (publications #5 and #1 below) and of ice (publication #6 below), the thermodynamic description of seawater is complete. In a real sense, the academic work required to address WG127's main objectives is virtually complete. The work remaining in order for WG127 to achieve its main goals is

- (i) To document its work in a way that will assist oceanographers to adopt these advances,
- (ii) to finalize the science and the algorithm that we recommend for the calculation of Absolute Salinity (reference #13, following on from #12)
- (iii) to write, test and describe suitable sets of computer algorithms that implement the new seawater thermodynamics,
- (iv) to assist IOC in the process of having all its member nations adopt the new practices for evaluating the thermodynamic properties of seawater, and to
- (v) assist and guide the oceanographic community leading up to the anticipated change in oceanographic practice on 1st January 2011.

Regarding point (iv) above we expect that in early 2009 IOC will establish an Evaluation Committee whose tasks will be

- (a) to read what WG127 is recommending as the new thermodynamic definition of seawater,
- (b) to decide whether the Absolute Salinity that WG127 is advocating is valid and appropriate,
- (c) to be cognisant of what IAPWS have already blessed through their official Release process, and
- (d) to decide whether the changes to oceanographic practice that WG127 are recommending are actually, on balance, worthwhile for the whole oceanographic community to adopt, and
- (e) to write a report to IOC for distribution to its member nations recommending the adoption of the new thermodynamic description of salinity and of seawater.

In Berlin we decided that in about April 2009 we would release on the web a Users Manual and software that would describe the new approach to thermodynamic measurements in oceanography, along with a web site at which the views of the community could be recorded. At the same time the IOC Evaluation Committee will be commissioned with the task of making a recommendation to IOC whilst taking into account the comments from the community that appear on the web site.

Over the next six months we need to continue working intensively on

- (i) the computer code and scientific paper that desceribes how Absolute Salinity is computed and
- (ii) the computer code that implement our findings based on the saline Gibbs function IAPWS-08
- (iii) writing both a scientific paper on the extra accuracy to be gained from using the new approach, and also a Users Manual for evaluating thermophysical properties in oceanography.

These tasks will keep us very busy until about April 2009. We anticipate that in the two years following this we will need to answer many practical questions that arise from the community consultation. (For example, one example that we are now considering is concerned with exactly what we recommed to instrument manufacturers. This issue is not entirely

straightforward since our previous community consultation has led us to recommend that national and international data bases continue to store Practical Salinity, while we will recommend that journals publish salinity as Absolute Salinity.)

Given that oceanographic practice will probably be changed to the new thermodynamics on 1st January 2011, we request that WG127 continue in its present form until 30 June 2011 so as to be a source of advice to SCOR, IAPSO and IOC on any issues that may arise concerning the practical implementation of the results of our existing activities. We recognise that this will mean that WG127 exists for much longer than a regular SCOR Working Group. However, it must also be recognized that our Working Group is rather unlike other working groups. While we have much work ahead of us, especially in the next year, there probably is no need for the full Working Group to meet again. There may well arise needs for meetings of a sub-set of Working Group members to finalize matters to do with the computer code and especially with the ways in which our recommendations are implemented by hardware manufacturers.

At the Berlin meeting in September 2008 IAPWS formed a new Subcommittee on "Seawater" with Rainer Feistel as chair. IAPWS have developed an interst in the thermophysical properties of seawater because of the use of seawater as cooling water in power stations and also because such properties are in demand for the operation of desalinition plants. Any future need for meetings of sub-groups of WG127 would sensibly occur in conjunction with the annual meetings of IAPWS (the next of which is at Arnhem, The Netherlands, 06 - 11 September 2009).

Other developments that occured at our working group meeting in Berlin include (i) in cooperation with PTB Braunschweig, high-precision density measurements (2 ppm) of standard seawater are planned to provide the oceanographic community with a novel, SI-traceable metrological salinity reference, so providing the community with an SI-traceable check on the (assumed) very accurate ampules of standard seawater that the oceanographic community currently uses to calculate salinity and to detect the slow drifts in salinity due to the melting of ice, and (ii) the real possibility that the Standard Seawater Service may publish the density of each batch of standard seawater along with its conductivity ratio, since it has become apparent that the vibrating tube densimeters represent a relatively accurate way of determining an absoulte value of the density of a fluid sample.

In summary, WG127 has been working hard over the past year, and we expect to be also running very fast in the coming year. It is encouraging to see many of our efforts maturing and to be well along the path to adoption. Since filing the annual report of progress of WG127 in July 2008, we have had our third meeting, and it has become apparent that it will take an extra year to get our work adopted by the international oceanographic community. This revised report reflects this revised timetable.

Trevor J McDougall Chair, SCOR/IAPSO Working Group 127

References

Note that of these 13 references all but #5 have been written by members of the SCOR/IAPWS WG127 (although the two IAPSO publications, #6 and #7, are not officially authored by individuals but by IAPWS itself). Four of the above publications were written prior to the formation of the Working Group; the remainder have arisen out of our on-going activities in WG127. Publications #5, #6 and #7 are the official thermodynamic descriptions of water vapour, liquid water, ice and seawater. The key papers that underlie the seawater Release (#7) are the WG127 publications #11 and #2. To use the new thermodynamic description of seawater one first needs to calculate Absolute Salinity and publications #12 and #13 are the only way of doing so.

- 1. Feistel, R., 2003. A new extended Gibbs thermodynamic potential of seawater. *Progress in Oceanography*, **58**, 43-114. This paper is an earlier version of paper #2 below.
- Feistel, R. 2009: A Gibbs Function for Seawater Thermodynamics for -6 to 80 °C and Salinity up to 120 g kg⁻¹. *Deep-Sea Research* I, **xx**, yyy-yyy, in press, available from Rainer Feistel at <u>rainer.feistel@io-warnemuende.de</u> and also from the web page <u>http://www.sciencedirect.com/science/journal/09670637</u> as an article "in press". This paper is the main science paper that represents the outcomes of WG127. The IAPWS-08 Release (paper #7 below) is the officially released version of this paper.
- 3. Feistel, R., Feistel, A., Guder, C., Jackett, D.R., Marion, G.M., Overhoff, U., Reissmann, J.H., Tchijov, V., Wagner, W., Wright, D.G., 2009. Numerical Implementation and Oceanographic Application of the Thermodynamic Potentials of Water, Vapour, Ice, and Seawater. *Ocean Science*, <u>in preparation</u>. This paper will be an on-line repository of all of the algorithms in several different computer languages. Many months of work remain to be done on this.
- 4. Feistel, R., D. G. Wright, K. Miyagawa, A. H. Harvey, J. Hruby, D. R. Jackett, T. J. McDougall and W. Wagner, 2009: Development of thermodynamic potentials for fluid water, ice and seawater: A new standard for oceanography. submitted to *Ocean Science* (and firstly to OSD). This manuacript is now "published" in *Ocean Science Discussions* and is available at <u>http://www.ocean-sci-discuss.net/5/375/2008/osd-5-375-2008.html</u>. This paper describes how the three different thermodynamic potentials of freshwater, ice Ih and the saline Gibbs function were made to be mutually self consistent. The paper lists the values of several key constants to twenty significant figures, and also many check values of the thermodynamic functions so that both double-precision and quadruple-precision numerical implementations can be unambiguously checked.
- 5. IAPWS, 1996. Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. The International Association for the Properties of Water and Steam. Fredericia, Denmark, September 1996. Internet: <u>http://www.iapws.org/relguide/IAPWS95.pdf</u> This is THE thermodynamic description of pure liquid water and pure water vapour. For good thermodynamic reasons it is in the form of a Helmholtz function (which has in situ density as one of its independent variables), which is a little inconvenient for oceanographic use. The paper Feistel (2003) [Ref #1] provides an alternative formulation for freshwater which oceanographers will mostly find more convenient, namely a Gibbs function of freshwater where the independent variables are the measured variables (salinity) temperature and pressure. IAPWS is planning for 2009 a Supplementary Release for Oceanographic Use of this 2003 Gibbs function.
- 6. IAPWS, 2006. Release on an Equation of State for H₂O Ice Ih. The International Association for the Properties of Water and Steam. Witney, UK, September 2006. Internet: http://www.iapws.org/relguide/Ice.pdf. This is THE thermodynamic description of the properties of ice Ih. It is the official IAPWS release based on the published research of Feistel and Wagner (2006). Ice Ih is the type of ice that is found in the oceanographic ranges of temperature and pressure.

- 7. IAPWS, 2008. Release on the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater. The International Association for the Properties of Water and Steam. Berlin, Germany, September 2008, available from Rainer Feistel at <u>rainer.feistel@io-warnemuende.de</u> and from <u>www.iapws.org</u> very soon. This is THE thermodynamic description of the saline Gibbs function, that is, the difference between the Gibbs function of seawater and the Gibbs function of freshwater. This is the officially checked Release of Feistel (2009), Ref #2.
- Jackett, D. R., T. J. McDougall, R. Feistel, D. G. Wright and S. M. Griffies, 2006: Algorithms for density, potential temperature, conservative temperature and freezing temperature of seawater. *Journal of Atmospheric and Oceanic Technology*, 23, 1709-1728. This paper is based on an older version of the Gibbs function of seawater. Ref #10 will be similar to this paper in that will provide an entry point for oceanographers to the work of WG127 and will summarize the increase in accuracy that comes from adopting the work of WG127.
- 9. McDougall, T. J., D. R. Jackett, D. G. Wright and R. Feistel 2003: Accurate and computationally efficient algorithms for potential temperature and density of seawater. *Journal of Atmospheric and Oceanic Technology*, **20**, 730-741. This paper was based on an earlier version of the seawater Gibbs function. Ref #10 will be similar to this paper in that it will provide an entry point for oceanographers to the work of WG127 and will summarize the increase in accuracy that comes from adopting the work of WG127.
- McDougall, T J, R Feistel, D R Jackett, B A King, G M Marion, F J Millero and D G Wright, 2009: Oceanographic application of the Gibbs function 2008 of seawater. <u>To be written</u>. For publication in *Deep-Sea Research I*. This paper will provide an entry point for oceanographers to the work of WG127 and will summarize the increase in accuracy that comes from adopting the work of WG127. It will outline what is recommended for the storage and use of salinity.
- Millero, F. J., R. Feistel, D. G. Wright and T. J. McDougall, 2008: The composition of Standard Seawater and the definition of the Reference-Composition Salinity Scale. *Deep-Sea Research* I, **55**, 50-72. also available from Frank Millero at <u>fmillero@rsmas.miami.edu</u>. This paper provides the rationale for the new definition of salinity, Absolute Salinity. To do so, the paper defines the composition of standard- or reference-seawater.
- 12. Millero, F. J., J. Waters, R Woosley, F. Huang and M. Chanson, 2008: The effect of composition on the density of Indian Ocean waters. *Deep-Sea Research I*, **55**, 460-470. also available from Frank Millero at <u>fmillero@rsmas.miami.edu</u>. This paper is the first to propose a practical expression for evaluating Absolute Salinity in terms of measured variables.
- 13. Millero, F. J., and unspecified co-authors, 2009: The effect of composition on the density and salinity in the global ocean. <u>To be written</u> by late 2008(?) *Deep-Sea Research I*, **xx**, yyy-yyy. This paper will provide an update to Ref #12, based on data from all the worlds' major ocean basins.

From 2008 IOC Executive Council Meeting (added by Ed Urban)

I-GOOS Chair's report included:

In September 2008 the SCOR–IAPSO Scientific Working Group 127 on "Thermodynamics and Equation of State of Seawater" will complete its work and a peer-reviewed update to the thermodynamic potential of standard seawater will be available to the oceanographic community for the first time since the currently used UNESCO standard (Fofonoff and Millard, UNESCO 1983: *Algorithms for computation of fundamental properties of seawater*,

UNESCO technical papers in marine science, 44) was universally adopted. The 25th Session of the IOC Assembly in 2009 will provide an opportunity to renew IOC's role as an international standard-setting body for oceanography, and for its 137 Member States to formally resolve to adopt the new standard.

Member State response report included:

Member States strongly supported presenting the Resolution concerning the SCOR–IAPSO Scientific Working Group 127 on "Thermodynamics and Equation of State of Seawater", to the 25th Session of the Assembly for its adoption as a universal standard.

Operative/Decision paragraph included:

The Executive Council **reaffirmed** IOC's commitment and **instructed** the Executive Secretary to work with the SCOR–IAPSO Scientific Working Group 127 with a view to presenting to the Assembly, at its 25th Session, the new Equation of State of Seawater, and to inviting the Assembly to adopt a Resolution to formally adopt this new standard.