Minutes of the joint meeting of TPWS/IRS/SCSW

Michael Hiegemann, Stockholm, June 30th

The session was opened by Alan Harvey. The agenda was corrected with addition of item 14.8 concerning a JCOMM intercomparison test (Pang) and item 14.9 on density standards at Anton Paar (Laky). During the discussion of item 13 the IRS will be discussing on the future of IRS. The agenda was adopted by the working groups.

Prof. Kretzschmar informed the attendees of Ines Stöcker, who passed away last week. Ines was involved in the preparation of several IAPWS papers and participated in several IAPWS meetings.

- 2. As Clerk of minutes were nominated: Jan Hruby for TPWS, Anuragh Singh for IRS and Michael Hiegemann for SCSW.
- 3. A
- 4. A
- 5. A
- 6. A
- 7. A
- 8. a
- 9. a

10. Humid air fugacity and enhancement factor (joint with SCSW)

10.1 Rainer Feistel reported on the work on a "Guideline on a virial equation for the fugacity of H2O in humid air". The fugacity is the most promising candidate to determine the relative humidity. The coefficients of the virial equation are derived analytically from the equations of state of air and water. The guideline comes with an estimate of the uncertainties.

10.2 Alan Harvey presented the results of evaluation task group on the above mentioned guideline. All numerical data was recomputed and compared to the data given in the guideline, with complete coincidence of all figures given. The guideline is considered complete and correct in its description and thus being recommended by adoption by the IAPWS executive committee.

10.3 Olaf Hellmuth reported on the "Determination of the enhancement factor and the saturated vapor mole fraction". There is an interest in this entity due to its influence of the global warming. The enhancement factor is determined as a virial approximation. The set of equations developed can be evaluated also using parts of the industrial formulation IAPWS-IF97 as the limits of application have been defined accordingly. The enhancement factor needs to be computed iteratively, and the paper comprises a method to determine starting guesses.

10.4 Olaf Hellmuth reported on behalf of a group (O. Hellmuth, R. Feistel, J. Lovell-Smith, J. Kalová, H.-J. Kretzschmar, S. Herrmann) suggesting next steps concerning the humid air properties. A virial approximation of the enhancement factor should be developed. Other topics discussed included an analytical approximation for the low-density water mole fraction in supercooled water (c.f. Item 17.1), an analytical correlation of the ratio of relative humidity to the relative fugacity, problems of metastable regions with respect to the suggested developments.

11. (MH not participating)

- 12. Reiner Feistel presented the results of the task group on the "Extension of range of formulation for thermodynamic properties of sea water". The report is an update of his talk at the IAPWS 2013 meeting. Data measurements will be finished by David Safarov In autumn 2015. The development of a new speed of sound sensor has been finished by Christoph von Rhoden and first data at atmospheric pressure has been measured; however his contract has come to an end and plans for further data are uncertain. The existing data could be included in a new correlation. Work on this correlation could start in spring 2016.
- 13. Collaboration with other international bodies (joint with SCSW):
 - 13.1 Rich Pawlowicz talked about work of the IAPWS/IAPSO/SCOR Joint Committee on Properties of Seawater (JCS). He presented an updated org chart of governmental and nongovernmental organizations in order to clarify where JCS could fit. The members and work groups of JCS are well defined. TEOS-10 is becoming a practically applied standard, indicated by the high number of software downloads and by the fact that there are several large climate models that have TEOS-10 support now. Ocean measurements are going on and focus on anomalies of salinity and of the chemical composition. The salinity/density subgroup are about to develop a best practice guide for high precision density measurements. The chemical composition of standard sea water is to be explored by pooling of experiences. The ph subgroup targets to write a more cook-book like document on the details of the creation of TRIS buffers. The Pitzer model is followed further. The relative humidity subgroup has written a technical report on the definition of Relative Humidity. The members of TPWS and SCSW support the directions taken by the work groups.

Reiner Feistel attended a Marine Instrument Workshop in China. Trevor McDougall was awarded the Australian Laureate Fellowship with a 2.7 AUS\$ funding over 5 years for the further development of thermodynamic tools and other instruments, i.e. to support TEOS-10.

13.2 The BIPM/IAPWS collaboration is ongoing and was presented by Reiner Feistel. The collaboration was initially triggered by the wish to develop an SI traceable salinity standard. The collaboration is being institutionalized by a position paper submitted to Metrologia in February 2015. It was decided to split the paper, such that there is a series of four papers and a substantial supplementary appendix now. The papers express a strong relation to climate research.

13.3 Reiner Feistel reported on a workshop with BIPM on measurement uncertainty in June 2015. The workshop was predominantly covering Bayesian Methods for the estimation of uncertainties to be part of a Guide to the expression of Uncertainty in Measurement (GUM). Reiner Feistel et al. have written a respective article on the uncertainty of correlated equations. The approach includes the requirement to publish the covariance matrix in addition to the coefficients of a correlation to enable the calculation of the errors. The new requirement will urge authors to apply a more rigorous analysis of the data published.

14. Sea water related topics (joint with SCSW):

14.1 Rich Pawlowicz presented work on the task "Best practices guide for density analysis". The guide shall encourage researchers to carry out more density measurements and is precise on all practical aspects from sample preparation to the execution of the measurement itself. There are some remaining issues on the sequence of measurements, concerning the linearity of the Anton-Paar measurement equipment and where to publish the document.

14.2 Hannes Schmidt explained the "Conductivity-density relation of standard seawater" in his talk. The uncertainty of the density measurement can be reduced by use of a substitution method in which alternating pure water and seawater samples are measured. This method is able to bring the uncertainty down to less than 2 g/m3 at atmospheric pressure and to less than 36 g/m3 for very high pressures. The measurement time is between 16 and 48 hours per point. The method is applicable from 5 to 35°C and up to pressures of 65 MPa. A number of possible sources of uncertainty were investigated.

14.3 The same speaker then reported on the "Seawater density comparison", targeting to compare vibrating tube densitometer measurements delivered by 11 groups. Some four results were analyzed in more detail, and it was found that corrections for aeration and for isotopic compositions need to be carried out consistently. After the execution of the corrections the results compared very well with the reference value from PTB.

14.4 Hiroshi Uchida discussed "Nonlinearities in seawater density measurements". Results of hydrostatic weighing are compared with calculated results from TEOS-10 and with measured results from the Anton Paar devices DMA5000M and DMA5000s (relative to pure water), where a correction for the results of the latter device has been recommended. There was a discussion about this nonlinearity correction, which Hannes had investigated thoroughly but found to be too small to worry about. However, the remaining alternative, that Standard Seawater had a density that differed from that described by TEOS-10, was not well received.

14.5 Rich Pawlowicz reported on "Density anomalies in coastal waters". TEOS-10 allows for variations of the chemical composition of sea water. Different areas not being "open ocean" were discussed, with a focus on river salt input. There is no generalization about major ions in rivers possible, but salinity anomalies can be correlated. However, the scatter about predictions involving river water is large. These remaining differences are systematical, and could result from sulphate reduction processes that do occur in sediments on shelves. However, there is no definite conclusion yet.

14.6 Reiner Feistel showed some slides on the GSW software toolbox. Version 3.05 was released in May 2015 and contains plenty of new programs. New ice functions have been added as well as a new function of specific volume.

14.7 He then reported on the IUPAC project on sea water pH, which is particularly concerning the activity of the H+ ion, described by a Pitzer equation. There is still a difference between the activity measured and the current Pitzer equation.

14.8 Yanan Li presented the NCOSM institute and their certification process. NCOSM is a government-run marine measurements institute in China. They recently carried out a JCOMM salinity intercomparison project. Two different types of sea water samples were prepared and shipped to 17 (?) different partner institutes. Only a few of the reported results differed considerable from the reference values.

14.9 Barbara Laky reported on the accreditation of the Anton Paar GmbH as a calibration laboratory for reference standard for density according to ISO 17025. The company is now accredited for a scope of liquid densities from 650 to 1550 kg/m3 at 15 to 40°C and at 1 atm. The smallest uncertainty is 20 g/m3.

15. New IAPWS sea water related documents (joint with SCSW):

15.1 Rich Pawlowicz, as chair of JCS, proposed the question "How do you maintain a standard?". The presentation contained information about proposed updates of the salinity anomaly algorithm and other algorithms in TEOS-10. Actually, TEOS-10 has changed in the past wrt the correction of errors and the replacement of some equations but the method for doing so was rather informal. A proposed formal procedure for implementing these improvements was sketched, resembling to practices in software engineering, reaching from paper publication, JCS involvement, formal agreement, beta version circulated to the JCS by an independent evaluator, and conversion of final beta to official version. Some changes to the initial proposal by Rich were included during the discussion in the meeting. There is a need for versioning and to archive older versions which are provided via the web page now. The formalization of the PSS-78 standard needs to be formalized and documented.

The formal procedure was then accepted by SCSW on behalf of IAPWS as the method by which TEOS-10 updates should be carried out.

15.2 Discussion on a supplementary release for a simplified density equation for oceanographic use. A task group was nominated, see below.

15.3 A task group headed by Rainer Feistel (further participants Rich Pawlowicz and Allan Harvey) was set up to list all IAPWS documents being part of TEOS-10, i.e. to describe the TEOS-10/IAPWS relationship, with the intention to write an Advisory Note. A further task group headed Rich Pawlowicz (further participants Trevor Mcdougall with co-opted expert Paul Barker) to prepare a supplementary release for a simplified equation of the density of water for oceanographic use. The respective evaluation task group is headed by Allan Harvey (further participants Rainer Feistel).

Finally, a discussion was held on the desirability of continuing cooperation between IAPWS and BIPM (leading to releases relevant to relative humidity problems) by meeting with the BIPM's CCT working group in Paris in April/May of 2016. The SCSW and TPWS WG agreed that a proposal should be put forward to the Executive to send an IAPWS representative from SCSW to this meeting, with an estimated cost of EUR1000.

Under new business was a continuation of item 13.3: A discussion between Reiner Feistel and Jan Hruby on the covariance method ended up in the proposal to set up a task group exploring the impacts of that method on IAPWS work. Members of the proposed task group are Reiner Feistel, Jan Hruby, Steffen Seitz, Jeremy Lovell-Smith, and Dan Friend.