## Minutes

## IAPWS Thermophysical Properties of Water and Steam WG

## Plzeň, Czech Republic, September 5-8, 2011

NOTE: These Minutes include many items that were held jointly with the IRS Working Group and/or the Subcommittee on Seawater (SCSW). Items are listed according to their order on the TPWS agenda, which is Attachment A. **Bold print** denotes significant actions.

1-2. The meeting was opened on Monday morning, September 5 by the TPWS Chair, Hans-Joachim Kretzschmar. The agenda (Attachment A) was adopted after minor additions (attachment reflects additions). The Chair noted that, in accordance with our procedure, the 2010 Minutes had been circulated and approved with minor corrections shortly after the 2010 meeting. Allan Harvey was appointed Clerk of Minutes for TPWS.

3. H.-J. Kretzschmar and G. Doleisch demonstrated access to a password-protected website for documents and presentations of the TPWS and IRS Working Groups and the SCSW. The site is accessible from the Working Groups page on www.iapws.org.

4. M. Anisimov discussed a proposed international collaboration between the group at the University of Maryland and the group of J. Hruby at the Academy of Sciences of the Czech Republic, on the topic of thermodynamic properties of supercooled water. The Working Groups endorsed the proposal.

5. (thermal conductivity) J. Sengers reported on the new correlation for the thermal conductivity of ordinary water, a joint effort with the International Association for Transport Properties. In addition to the correlation for general and scientific use, the release also contains instructions for industrial use. R. Mareš presented the report of the evaluation of both the general/scientific formulation and the modification for industrial use, with a favorable recommendation. The Working Groups TPWS AND IRS voted to approve the Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance and to recommend that the EC send it out for Postal Ballot following review by the Editorial Committee. Prof. Kretzschmar, on behalf of the Working Groups, will send letters of appreciation to Dr. Huber at NIST and to Mr. Miyagawa thanking them for all their excellent work on this project.

H.-J. Kretzschmar presented a report on behalf of Mr. Miyagawa on the consequences on viscosity and thermal conductivity calculations in the industrial Region 3 if the density is obtained not by iteration but rather by the v(p,T) backward equations. This procedure is very accurate for viscosity; for thermal conductivity there is a small region where significant accuracy is lost.

6. (properties at 0.1 MPa) A. Harvey presented a proposed revision of the supplementary release on properties of liquid water at 0.1 MPa, changed only to reflect the new thermal conductivity formulation. H.-J. Kretzschmar presented the favorable test report on behalf of Mr. Miyagawa. The Working Groups TPWS AND IRS voted to approve the Revised Supplementary Release on Properties of Liquid Water at 0.1 MPa and to recommend that the EC send it out for Postal Ballot following review by the Editorial Committee.

7. (Industrial steam property calculations) (this item is reported in the IRS Minutes).

8. (humid air, CCS technology) (<u>the first 2 talks under this item are reported in the PCC Minutes</u>) (<u>the remainder</u> of this item is reported in the IRS minutes).

9. (seawater for industrial use) J. Cooper, as Chair of the Task Group, reported that no progress had been made during the year. A document (Guideline or Advisory Note, to be decided) will be prepared and circulated in time to discuss at the 2012 meeting.

#### 10. (seawater) (these items are reported under item #8 in the SCSW Minutes)

11. (dew point of combustion gases) (this item is reported in the IRS Minutes)

12. (metastable steam and nucleation) J. Hruby explained the expiring ICRN-15 on thermodynamic properties of metastable steam and gave some reasons why it had not produced the data hoped for. He has prepared a closing statement, and the WGs endorsed closing the ICRN with this statement. He then presented a draft for a replacement ICRN with a broader scope. The WG voted to recommend (subject to minor editing) sending the new ICRN "Thermophysical Properties of Metastable Steam and Homogeneous Nucleation" for consideration by the National Committees.

13. (supercooled water) V. Holten presented the status of an ongoing project to produce a better description of the thermodynamic properties of supercooled water.

14. (molecular simulations, joint with PCAS) O. Marsalek, N. Matubayasi, and K. Yasuoka presented their molecular simulation work, with titles described in the Agenda.

15. (IAPWS/BIPM collaboration) R. Feistel gave a report on this issue, describing the overlap of interests and possible areas of cooperation, and some of the questions that need to be answered. TPWS and SCSW decided to appoint several individuals to help in deciding what the initial letter from IAPWS to BIPM should say; these were J. Cooper, R. Feistel, D. Friend, A. Harvey, O. Hellmuth, H.-J. Kretzschmar, and P. Spitzer.

16. (16th ICPWS) J. Cooper briefly described a tentative list of topics for the 2013 ICPWS in the UK. Any comments from WG members were asked to be given to him by noon Wednesday.

17. (IAPWS-95 at low temperatures) R. Feistel reported that a method had been developed to extend the ideal-gas heat capacity formulation that was used in IAPWS-95, making its lower limit 50 K instead of 130 K with no change in IAPWS-95 itself. W. Wagner suggested minor editorial changes in the IAPWS-95 document to clarify its use for the low-temperature gas. It was agreed (with one negative vote) to authorize the proposed editorial changes, consisting of changing a mention of 200 K for extrapolation in this region to 130 K, deleting the following sentence, and updating the corresponding reference. R. Feistel, W. Wagner, and I. Weber were appointed as a Task Group to prepare a Guideline for 2012 on use of IAPWS-95 from 50 K to 130 K, and to consider if an editorial change is needed for the metastable region of IAPWS-IF97. The TPWS Chair may appoint an Evaluation Task Group during the year if a draft is prepared sufficiently before the 2012 meeting.

18.1. Regarding the requested Mission Statement, the following minor modification of the statement adopted last year was agreed on:

To develop state-of-the-art formulations for the thermophysical properties of water (in all its phases) and important water-containing mixtures as needed for scientific and industrial applications, and to encourage and facilitate research to improve knowledge of these properties.

18.2. A. Harvey reported that very recently CODATA had issued an update of the fundamental physical constants, and that there were also some recent new recommendations from IUPAC about molecular weight to be considered. A report and recommendations for changes to the Fundamental Constants document will be prepared for the 2012 meeting.

18.3. A. Harvey and J. Cooper reported that a few minor editorial revisions were needed to complete the document approved at the 2010 meeting. They were authorized to make these revisions and update the document.

18.4. TPWS supported the proposed revision to the By-Laws.

18.5. TPWS appointed Prof. Koichi Watanabe to be its representative to the Gibbs Award committee.

18.6. I. Weber reported that the Advisory Note Task Group appointed in 2010 had not made any progress. The following changes were made in its membership: M. Hiegemann is the new Chair, P. Murphy is added as a member.

18.7,8. A. Harvey presented the recommendation of the Task Group formed by the EC to investigate links to live table calculations hosted elsewhere. K. Orlov presented a modification of the proposal and demonstrated how it would look on the Russian site. The WG endorsed this recommendation for providing these links (with disclaimer) on the IAPWS website.

18.9. H.-J. Kretzschmar reported on the availability from his institute of free steam tables for Excel, Mathcad, and for pocket calculators.

18.10. J. Cooper stated that there was nothing new to report regarding liaison with the IEC.

18.11. This item was postponed.

19. Regarding collaborative projects, no further WG action is required.

# 20. The WG approved the addition of J. Kalová (University of West Bohemia, Czech Republic), V. Vinš (Institute of Thermomechanics, Czech Republic), and O. Hellmuth (Leibniz Institute for Tropospheric Research, Germany) to membership in TPWS.

21. The Chair of TPWS, Prof. Kretzschmar, will step down at the conclusion of the 2011 meeting. Dr. Harvey, currently a Vice-Chair, stated his willingness to become Chair at that time. It was voted to recommend to the EC that Dr. Harvey become Chair of TPWS, effectively immediately after this meeting, and that Dr. Hruby remain Vice-Chair.

22/23. The Chair and Clerk of Minutes were appointed to prepare the contribution to the Press Release and the formal motion of the TPWS WG to the EC.

24. The meeting was adjourned at 5:15 PM on Thursday, September 8.

## Agenda for the Working Group

## Thermophysical Properties of Water and Steam (TPWS) Plzeň, Czech Republic, 04-09 September 2011

- 1. Opening Remarks; Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. OPAL Web Space for Working Material for WGs TPWS, IRS, and SC SW, joint with WG IRS and SC SW (G. Doleisch, H.-J. Kretzschmar)
- 4. Potential International Collaborative Projects
- 5. Release on the IAPWS Formulation 2011 for the Thermal Conductivity of Ordinary Water Substance, joint with WG IRS and SC SW
  - Report (J.V. Sengers, E. Vogel, R.A. Perkins, M.L. Huber, D.G. Friend, M.J. Assael, I.N. Metaxa)
  - Test Report on the Scientific Formulation (R. Mares, J. Hrubý, K. Miyagawa, V. Vinš, K. Orlov)
  - Test Report on the Industrial Formulation (W.T. Parry, J. Hrubý, K. Miyagawa, V. Vinš, K. Orlov)
  - Formal consideration of the Release
  - Additional Test Report on Using Backward Equations v(p,T) of IAPWS-IF97 Region 3 for Calculating Thermal Conductivity (K. Miyagawa, H.-J. Kretzschmar)
- 6. Revised Supplementary Release on Properties of Liquid Water at 0.1 MPa, joint with SC SW and WG IRS
  - Report (A.H. Harvey)
  - Test Report (K. Miyagawa, H.-J. Kretzschmar)
  - Formal consideration of the Revised Supplementary Release
- 7. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG IRS (Tuesday 08:30 am)
  - 7.1 Report of the Industrial Requirements Task Group (I. Weber, W.T. Parry)
  - 7.2 Report of the Industrial Survey Task Group (W.T. Parry)
  - 7.3 Using IAPWS Formulations in Power Cycle Calculations with the Program EBSILON (R. Pawellek, P. Krueger, STEAG Energy Services Zwingenberg, Germany)
  - 7.4 Steam Property Calculations for CFD Applications (P.J. Murphy)
  - 7.5 Implementation of TTSE in Power Plant Transient Simulation Software Experiences and Results (H. Steuer, J. Bonifay, Siemens Energy Erlangen, Germany)
  - 7.6 Other Backward Equations with Different Independent Variables for IAPWS-IF97 (J. Cooper)

- 8. Properties of Humid Air and Humid Combustion Gases for CCS Technology, joint with WGs IRS, PCAS, PCC and SC SW (Tuesday 01:30 pm)
  - Thermodynamic Modeling of Processes Related to Carbon Dioxide Capture and Sequestration (A. Anderko)
  - Development of Thermodynamic Models for Hydrates in Water–Carbon Dioxide Mixture (V. Vinš, A. Jäger, J. Gernert, J. Hrubý, R. Span)
  - Closing Statement for ICRN-14 (A.H. Harvey, R. Span)
  - Proposal for a new ICRN (R. Span, A.H. Harvey)
- 9. Guideline on the Properties of Sea Water for Industrial Use, joint with WGs IRS and SC SW (Tuesday 1:30 pm, after joint session with PCC)
  - Report of the Task Group (J. Cooper, R. Feistel, M. Hiegemann)
- 10. Properties of Seawater (R. Feistel), joint with SC SW and partly with WG IRS (Tuesday 1:30 pm, after joint Session with PCC)
  - 10.1 Implementation of the TEOS-10 Libraries (T.J. McDougall, P. Barker, R. Feistel, J. Reissmann)
  - 10.2 New Seawater Measurements (R. Feistel, F.J. Millero, J. Safarov, A. Heintz, E. Hassel)
  - 10.3 Regular Measurement of Seawater Density with Anton Paar Instruments (B. Laky, S. Weinreben, R. Feistel)
  - 10.4 Task Group Report "Industrial Requirements" (M. Hiegemann, J. Bellows, H. Glade)
  - 10.5 Task Group Report "Transport Properties" (A. Anderko) Available Technical Report: Wang, P, Anderko, A.: Modeling Thermal Conductivity of Electrolyte Mixtures in Wide Temperature and Pressure Ranges: Seawater and Its Main Components.
  - 10.6 Electrical Conductivity of Seawater (R. Feistel, R. Pawlowicz)
  - 10.7 Solubility of CO<sub>2</sub> in Seawater (J. Safarov)
  - 10.8 On the Definition of Relative Humidity (R. Feistel, J. Lovell-Smith)
- 11. Dew Point of Combustion Gases, joint with WGs IRS, PCAS, and SC SW (Thursday 08:30 am)
  - Report on new Dew Point Equations and Status of ICRN-23 (N. Okita)
- 12. Metastable Steam and Nucleation, joint with WGs IRS, PCAS, and SC SW (Thursday 08:30 am)
  - Report of the Task Group (J. Hrubý, K. Yasuoka, N. Okita)
  - Discussion about ICRN 15, expires September 2011
- 13. Properties of Supercooled Water, joint with PCAS and SC SW (Thursday 08:30am)
  - Peculiar Thermodynamics and Equation of State for Supercooled Water (V. Holten, C.E. Bertrand, J. Kalova, D. Fuentevilla, M.A. Anisimov, and J.V. Sengers) Available Technical Reports: Holten, V., Bertrand, C.E., Anisimov, M.A., Sengers, J.V., Thermodynamic Modeling of Supercooled Water. Kalova, J., Mares, R., Anisimov, M.A., Sengers, J.V., Scaled Equation of State for Supercooled Water in the mean-field Approximation.

- 14. Molecular Simulations, joint with PCAS (Thursday 08:30 am)
  - 14.1 Structure, dynamics and reactivity of the hydrated electron (O. Marsalek, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic)
  - 14.2 Molecular study of hydration over a wide range of thermodynamic conditions (N. Matubayasi)
  - 14.3 Molecular dynamics simulation of vapor/liquid coexistence for water and methane/water (K. Yasuoka)
- 15. Suggestions for IAPWS BIPM Collaboration, joint with SC SWReport (R. Feistel, S. Rudtsch)
- 16. Discussion of Main Topics for the 16th ICPWS 2013 in London (H.-J. Kretzschmar, A.H. Harvey, J. Hrubý), joint with WG IRS and SC SW
- 17. Editorial Changes on the IAPWS-95 Release and a Guideline on a Low-temperature Extension of IAPWS-95 (R. Feistel, W. Wagner)
- 18. Reports on Other TPWS, IRS and SC SW Activities
  - 18.1 Revision of the Mission Statement of WG TPWS (H.-J. Kretzschmar, A.H. Harvey)
  - 18.2 Guideline on Fundamental Constants (A.H. Harvey), joint with WG IRS and SC SW
  - 18.3 Update of Advisory Note # 2: Roles of Various IAPWS Documents (J.R. Cooper, A.H. Harvey), joint with WG IRS and SC SW
  - 18.4 Changes of IAPWS Statutes and By-Laws (A.H. Harvey)
  - 18.5 Nomination of a TPWS Representative for Gibbs Award Committee (H.-J. Kretzschmar, A.H. Harvey)
  - 18.6 Report of the Advisory Note Task Group (I. Weber, W.T. Parry)
  - 18.7 Web presentation of Releases, etc. (A.H. Harvey), joint with WG IRS and SC SW
  - 18.8 Links to Live Calculations of IAPWS Releases on IAPWS Website (K.A. Orlov, V.F. Ochkov), joint with WG IRS and SC SW
  - 18.9 Steam Tables for Excel<sup>®</sup>, Mathcad<sup>®</sup>, and Pocket Calculators for Education on the IAPWS Website (H.-J. Kretzschmar), joint with WG IRS
  - 18.10 Liaison with IEC (J.R. Cooper), joint with WG IRS
  - 18.11 Discussion about IAPWS Meetings Regarding Locations and Costs (H.-J. Kretzschmar), joint with IRS and SC SW
- 19. Other Business
  - Report on International Collaborative Projects
- 20. Membership
- 21. Election of new Chair
- 22. Preparation of contribution to Press Release
- 23. Preparation of the Formal Motion to the EC
- 24. Adjournment