Minutes: IAPWS Thermophysical Properties of Water and Steam WG
Stockholm, Sweden, 29 June – 2 July 2015

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.

Obituary: H.-J. Kretzschmar reported that Dr. Ines Stöcker, member of TPWS, died in June at the age of 53. Ines Stöcker participated in several IAPWS projects: the development of IAPWS-IF97, four supplementary releases to IF-97, advisory notes No. 3 (Thermodynamic Derivatives) and 5 (Industrial Calculations for Seawater). She was involved in organizing the 15th ICPWS in Berlin. She attended many IAPWS Meetings and conferences starting from 1995 in Paris. The WGs observed a minute of silence in remembrance of Dr. Stöcker.

1-2. The meeting was opened on Monday, June 29 by the TPWS Chair, Allan Harvey. The agenda (Attachment A) was adopted after some additions. The Chair noted that the 2014 Minutes had been circulated and approved with shortly after the 2014 meeting. J. Hrubý was appointed Clerk of Minutes for TPWS. (Michael Hiegemann was appointed Clerk for SCSW and Anurag Singh for IRS)

3. Mathias Kunick informed about the OPAL Web Space for sharing the working material of WGs.

4. Collaborative project "Towards an IAPWS Guideline for the Thermodynamic Properties of Supercooled Heavy Water" was proposed by M. A. Anisimov and J. Hrubý. Besides developing a new formulation for the region of cold and supercooled heavy water, the project should also provide information for the present development of the fundamental equation of state of heavy water. **TPWS unanimously recommended the Project for being granted.**

5. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG IRS

5.1 Report of the Task Group "Industrial Advisory Note" (M. Hiegemann, B. Rukes, A. Singh, A. Harvey) – see IRS Minutes

6. Proposal for an IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using Spline Interpolation, joint with WG IRS – see IRS Minutes

TPWS and IRS voted unanimously to approve the technical content of the IAPWS Guideline on the Fast Calculation of Water and Steam Properties in Computational Fluid Dynamics Using Spline Interpolation and to recommend that it be sent for Postal Ballot by the EC after editorial revisions.

7. Heavy Water Properties, joint with WG IRS

7.1 A. Harvey reported on behalf of the Task Group on Heavy Water Thermodynamic Properties (R. Span, A. Harvey, S. Herrig, E. Lemmon). An equation of state of heavy water has been developed with the aim of replacing the present formulation of thermodynamic properties of heavy water developed by Hill (1982, 1983). The new equation has only 24 terms and shows plausible extrapolation behavior. New data has been included (e.g., speed of sound by Wegge and Span). A further potential improvement would introduce new data for the ideal-gas properties (see item 17.4), and there may be additional vapor pressure and/or virial coefficient data. Because of the uncertainty of timing of new data, it is not clear when the equation will be finalized.

7.2 A. Harvey reported on behalf of the TG for Heavy Water Transport Properties (J. Sengers, M. Assael, M. Huber (co-opted expert), A. Harvey). Experimental data has been collected by M. Assael. R. Hellmann (Rostock) will calculate dilute-gas viscosity and thermal conductivity. Calculated values will be used together with experimental data. R. Perkins of NIST was approved by the TPWS and IRC WGs as another "Coopted Expert" for the Task Group.

8. V. Vinš reported on the progress of the Task Group on Surface Tension of Ordinary Water (joint with WG IRS and SC SW) (V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, J. Kalová, R. Mareš). Review and analysis of both old and new literature data, further measurements for supercooled water. 2016 – revision of the uncertainty measurements, 2017 – development of a new correlation. V. Vinš further reported on new measurements of the surface tension of supercooled water. The new data agree with the IAPWS formulation, except for the lower temperature limit, where the measured values are about 0.2% higher (almost within the experimental uncertainty). J. Kalová reported on the values of surface tension at 20 and 25 °C.

9. W. Wagner reported on a study by himself and M. Thol on the behavior of IAPWS-95 from 250 K to 300 K and up to 400 MPa. The evaluation was based primarily on newly evaluated speed of sound data by Lin and Trusler. An improved equation was fitted to the speed of sound data. The results are in agreement with the equation by Holten et al. (proposed for IAPWS Guideline under Item 11). The evaluation enables to provide estimates for the uncertainty of the isobaric heat capacity close to the melting line at high pressures. **A task group (W. Wagner, A. Harvey) was formed to include the new estimates into the IAPWS-95 release.**

10. Humid Air Fugacity and Enhancement Factor, joint with SC SW.

10.1 R. Feistel reported on behalf of the proposers of "Guideline on a Virial Equation for the Fugacity of H_2O in Humid Air" (R. Feistel, O. Hellmuth, J. Lovell-Smith). The Guideline provides an explicit expression for the fugacity of water vapor in air which is based on literature correlations for the temperature dependency of virial coefficients of the water vapor – air system.

10.2 A. Harvey presented the Report of the Evaluation Task Group (A. Harvey, H.-J. Kretzschmar). They found that the Draft Guideline is correct and recommended it for approval.

10.3 **TPWS and SCSW unanimously recommended that the Guideline be approved by the EC.**

10.4 O. 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 may be developed, and maybe a correlation based on structural optimization. Other topics discussed included an analytical approximation for the low-density water mole fraction in supercooled water (c.f. Item 11.1), an analytical correlation of the ratio of relative humidity to the relative fugacity, problems of metastable regions with respect to the suggested developments.

11. Metastable Water (joint with SC SW)

11.1 M. Anisimov presented on behalf of the proposers the background of supercooled water Guideline (V. Holten, M. Anisimov, J. Sengers). The formulation is based on an idea of two competing structures of liquid water which are represented in a quasi-chemical formalism. This view of the supercooled water has been partly confirmed by experiments. The formulation is valid up to 400 MPa and down to the homogeneous ice nucleation limit. It can be extrapolated to negative pressures down to -50 MPa.

11.2 J. Hrubý reported on behalf of the Evaluation Task Group on Supercooled Water Guideline. The formulation did not change since the Moscow meeting 2014, where a detailed report was presented including the issues of representation of experimental data, consistency with IAPWS-95 in the region of overlap, and physical correctness. Therefore, these issues were not re-iterated by the Task Group. Only formal changes have been suggested by the Task Group and they were adopted by the Proposers. The Task Group recommended the Guideline for adoption.

11.3 **TPWS and SCSW unanimously recommended the Guideline on Thermodynamic Properties of Supercooled Water for adoption by the EC.**

11.4 O. Hellmuth reported on behalf of the Task Group on Supercooled Water ICRN (O. Hellmuth, V. Holten, J. Sengers, J. Hrubý). The ICRN stimulates new experimental data for thermophysical properties of supercooled water.

11.5 **TPWS and SCSW unanimously recommended the ICRN (ICRN 30: Thermophysical Properties of Supercooled Water) and requests that the EC send it to be voted on after the meeting by the procedure specified in the By-Laws.**

The topic of interfaces of supercooled water is important, but was excluded from this ICRN. **A Task Group on an ICRN for Interfacial Properties of Supercooled Water was appointed, consisting of O. Hellmuth, J. Hrubý, and J. Sengers.**

11.6 M. Duška reported on behalf of the group of J. Hrubý on the progress of measurements of density of supercooled water at elevated pressures. New apparatus for measurements of the density of supercooled liquids has been developed showing reproducibility of 0.01% in density. Preliminary data from -20 to 20°C and from 0.1 MPa to 100 MPa agrees well with data by Sotani and with the IAPWS Guideline.

11.7 H.-J. Kretzschmar left the Task Group on Superheated liquid water. The Task Group did not have any output. In a consequent discussion it was concluded that such a Task Group is needed. The remaining task group (J. Hrubý and R. Feistel) will continue.

11.8 A. Harvey reported on behalf of the Task Group on possible revision of IAPWS formulations for melting curves (V. Holten, A. Harvey, H.-J. Kretzschmar). Formulation is not yet available. In the discussion it has been confirmed that new formulations are needed as it is clear that better results can be achieved. The Task Group hopes to have a proposal for 2016.

12. Report of Task Group on Extension of Range of Formulation for Thermodynamic Properties of Sea Water, joint with WGs IRS and SC SW (R. Feistel) – see SCSW minutes

13. Cooperation with other international bodies, joint with SC SW – see SCSW minutes

14. Reports on seawater-related topics, joint with SCSW – see SCSW minutes

15. Proposed new IAPWS seawater-related documents (joint with SCSW) – see SCSW minutes

16. Reports on miscellaneous TPWS scientific topics (joint with WG IRS)

16.1 K. Meier reported on thermophysical property research at Helmut-Schmidt-University in Hamburg. Founded in 1973 as one of two universities of the armed forces, good conditions for performing experimental research. The research concerns thermophysical properties of fluids, mass transport across fluid interfaces, and heat transport in gas turbines. Experimental apparatuses include pulse-echo speed of sound instrument for liquids, automated vibrating tube densimeter, torsional crystal viscometer, combined vibrating wire viscometer and magnetic suspension balance densimeter for gases.

16.2 E. E. Ustyuzhanin reported on a comparative study of Ps(T) models for H_2O in the critical region (E. E. Ustyuzhanin, V. F. Ochkov). Cosiderations have been presented concerning the critical scaling of the two-phase heat capacity of water and the second derivative of the saturated vapor pressure with respect to temperature. Extrapolation of the IAPWS-IF97 equation for saturation vapor pressure towards the critical point was investigated.

16.3 V. Ochkov reported on the online calculation from IAPWS formulations (V. Ochkov, K. Orlov). Elsevier publishes reference books in the Knovel series enabling computations in their electronic editions. Online computations based on IAPWS computations have been implemented at the Knovel web site. A printed handbook for thermal computations is available.

16.4 M. Hiegemann suggested an innovative concept for fluid property approximations. He reviewed the current methodology for structural optimization of thermophysical property formulations. Slow evaluation, complex structure, non-generic – different structure for each fluid. Chebychev polynomials Clenshaw algorithm for a fast evaluation. Two variants for Semi-infinite transform have been presented. An application to the isobaric ideal gas heat capacity based on Woolley data enabled fitting within 0.02% in a range from 130 to 2000 K with 13 terms.

17. Joint session with WG PCAS

17.1 Report of Task Group on Transport Properties of Seawater, joint with SC SW and WG IRS

A. Anderko reported on behalf of the proposers of the Guideline on Thermal Conductivity of Seawater. The guideline is based on a correlation originally developed for atmospheric pressure, which has been extended by the pressure dependence. Originally, the formulation was expressed in terms of individual ionic species. Based on the previous Evaluation Task Group suggestions, the formulation was simplified such that the effect of solutes is expressed in terms of the absolute salinity.

17.2 R. Pawlowicz reported on behalf of the Evaluation Task Group for Seawater Thermal Conductivity. He reported about the tests performed. The Evaluation Task Group recommended to accept the Guideline.

17.3 **TPWS, SCSW, and IRS unanimously recommended the Guideline on Thermal Conductivity of Seawater to be approved by the EC.**

17.4 J. Hrubý reported on the progress toward improved ideal-gas properties of ordinary and heavy water (J. Hrubý, A. Harvey). Very accurate data for the partition function and related thermodynamic properties in the ideal gas state are available (Prof. A. Császár, Budapest) for the most abundant isotopologue $H_2{}^{16}O$, their uncertainties are being considered. Preliminary data for deuterated isotopologues have been provided. Deviations on the order of 1% from the present heavy water ideal-gas formulation have been observed (so this work will contribute to improving the new heavy water equation of state). In a discussion it was suggested that the differential evaporation of various isotopologues should be investigated. **A task group including D. Friend, R. Feistel and J. Hrubý has been formed to come up with an opinion of whether this topic is relevant for IAPWS.**

17.5 A. Harvey reported on the progress in the development of first-principles data to extend knowledge of the second virial coefficient of ordinary and heavy water (A. Harvey, G. Garberoglio, P. Jankowski, K. Szalewicz). Computations have been performed using newly developed potentials using classical, semi-classical, and full quantum, path integral approaches. The computed data enable to extend the temperature range for the 2nd virial coefficient for both H_2O and D_2O to lower and higher temperatures. Classical computations are in error already at quite high temperatures. Semi-classical computations provide correct second virial coefficients at least down to 300 K. This work will, among other things, provide 2nd virial coefficients to help the fit of the new formulation for thermodynamic properties for D_2O.

17.6 H. Miyamoto reported about modeling thermodynamic properties of mixtures of natural substances used as working fluids for heat pumps and organic Rankine cycle (H. Miyamoto, R. Akasaka, E. Lemmon). Four apparatuses were used to investigate thermophysical properties for isopentane. bellows volumeter 200 MPa, 600 K. Small sample, completely sealed.

18. IAPWS Certified Research Needs (ICRNs) – reported by A. Harvey

18.1 ICRN 27: Thermophysical Properties of Humid Gases and CO_2-Rich Mixtures - closing statement will be prepared by R. Span and A. Harvey. An ICRN on CCS-related research will be considered.

18.2 ICRN24: Thermal Conductivity of H_2O at Low Pressures and High Temperatures. New theoretical data have been prepared by R. Hellmann (Rostock). Since the IAPWS thermal conductivity formulation is finished, it was felt that there was no urgent need for further research, so the ICRN should be allowed to expire. A. Harvey will prepare a closing statement.

19. Reports on other TPWS activities

19.1 A. Harvey reported on the status of the Guideline on Fundamental Constants. No updates have been prepared. An update for the Vienna standard for ordinary water will possibly have an impact on the Guideline.

19.2 A. Harvey reported on the Advisory Note 2 (J. Cooper, A. Harvey). The Guidelines on supercooled water and on the spline-based table lookup method will be added and other aspects will be brought up to date.

20. Other Business

20.1 Report on International Collaborative Projects – no collaborative projects in the past year. See item 4 for a new proposal.

20.2 Discussion of IAPWS document numbering/designation. Various opinions have been expressed. Possibility of DOI numbering has been discussed. Editorial committee will prepare a suggestion.

20.3 Topics for 2018 ICPWS have been discussed. No new symposia have been suggested; members are encouraged to send ideas for sessions to J. Hrubý in the next few months. The conference will be prepared on the basis of 16th ICPWS in London.

21. Membership

Membership in TPWS has been terminated for Dr. Johannes Gernert (formerly of Ruhr Universität Bochum, Germany) because a change in his professional career does not allow him to follow the TPWS activities, and for Dr. Petra Spitzer who has retired from the PTB. Membership of Dr. Ines Stöcker ceased as she passed away.
Two proposals were submitted for TPWS membership: Dr. Hiroyuki Miyamoto (Toyama Prefectural University, Japan) and Prof. Dr. Ing. Karsten Meier (Helmut-Schmidt-University in Hamburg, Germany). Both proposals were unanimously approved by the Working Group.

22. Contribution to Press Release
The chair and the clerk of minutes were assigned to prepare the contribution to the Press Release.

23. Preparation of the Formal Motion to the EC
The chair and the clerk of minutes were assigned to prepare the Formal Motion to the EC.

24. Adjournment
The meeting was adjourned at 2:15 p.m. on Thursday, July 2.

Preliminary Agenda for the IAPWS Working Group: Thermophysical Properties of Water and Steam (TPWS)

Stockholm, Sweden, 29 June - 2 July 2015

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 (H.-J. Kretzschmar)
4. Potential International Collaborative Projects [Monday]
5. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG IRS [Monday]
   - 5.1 Report of the Task Group "Industrial Advisory Note" (M. Hiegemann, B. Rukes, A. Singh, A. Harvey)
6. Proposal for an IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using Spline Interpolation, joint with WG IRS [Monday]
   - 6.1 Report of proposers (H.-J. Kretzschmar, M. Kunick, J. Hrubý, M. Duška, V. Vinš, F. di Mare, A. Singh)
   - 6.2 Report of Evaluation Task Group (A. Novy et al.)
   - 6.3 Formal consideration of the Guideline
7. Heavy Water Properties, joint with WG IRS [Monday]
   - 7.1 Report of Task Group on Heavy Water Thermodynamic Properties (R. Span, A. Harvey, S. Herrig)
   - 7.2 Report of TG for Heavy Water Transport Properties (J. Sengers, M. Assael, M. Huber; reported by A. Harvey)
8. Report of Task Group on Surface Tension of Ordinary Water (joint with WG IRS and SC SW) (V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, J. Kalova, R. Mareš) [Monday]
9. Behavior of IAPWS-95 from 250 K to 300 K and up to 400 MPa: Evaluation Based on Recently Derived Property Data (W. Wagner, M. Thol) [Monday]
10. Humid Air Fugacity and Enhancement Factor, joint with SC SW
    - 10.1 Report of the proposers of "Guideline on a Virial Equation for the Fugacity of H_2O in Humid Air" (R. Feistel, O. Hellmuth, J. Lovell-Smith)
    - 10.2 Report of the Evaluation Task Group (A. Harvey, H.-J. Kretzschmar)
    - 10.3 Formal consideration of the Guideline by the Working Groups
    - 10.4 Next steps: Determination of the enhancement factor and saturated water vapor mole fraction (O. Hellmuth, R. Feistel, J. Lovell-Smith, J. Kalova, H.-J. Kretzschmar, S. Herrmann)
11. Metastable Water (joint with SC SW) [Tuesday]
    - 11.1 Background of supercooled water Guideline (V. Holten, M. Anisimov, J. Sengers)
    - 11.2 Report of Evaluation Task Group on Supercooled Water Guideline (J. Hrubý)

11.3 Formal consideration of the Guideline by the Working Group

11.4 Report on Task Group on Supercooled Water ICRN (O. Hellmuth, V. Holten, J. Sengers, J. Hrubý)

11.5 Formal consideration of Supercooled Water ICRN

11.6 Progress of measurements of density of supercooled water at elevated pressures (M. Duška, J. Hrubý)

11.7 Report of Task Group on Superheated liquid water, joint with WG IRS and SCSW (H.-J. Kretzschmar)

11.8 Report of Task Group on possible revision of IAPWS formulations for melting curves (V. Holten, A. Harvey, H.-J. Kretzschmar)

12. Report of Task Group on Extension of Range of Formulation for Thermodynamic Properties of Sea Water, joint with WGs IRS and SC SW (R. Feistel) [Tuesday]

13. Cooperation with other international bodies, joint with SC SW [Tuesday]

13.1 IAPWS/IAPSO/SCOR Joint Committee on Seawater, including updates to TEOS-10 (R. Pawlowicz)

13.2 Metrologia article on BIPM/IAPWS interaction (R. Feistel)

13.3 Cooperation with BIPM (Uncertainty Workshop) (R. Feistel)

13-IRS Separate IRS meeting for IRS future discussion (I. Weber).

14. Reports on seawater-related topics, joint with SCSW [Tuesday]

14.1 Best practices guide for density analysis (H. Wolf, S. Weinreben, H. Uchida, R. Pawlowicz)

14.2 The Conductance-Density Relation of Standard Seawater (Schmidt, Wolf)

14.3 Seawater Density Comparison (Schmidt, Wolf)

14.4 Nonlinearities in Seawater density measurements (Uchida)

14.5 Density anomalies in coastal waters (R. Pawlowicz, H. Uchida, F. Millero)

14.6 Update on GSW software toolbox (Feistel and Barker)

14.7 Update on seawater pH (Feistel and Camoes)

14.8 JCOMM intercomparison (Pang)

14.9 Density standards at Anton Paar (Laky)

15. Proposed new IAPWS seawater-related documents (joint with SCSW) [Tuesday]

15.1 Discussion on Guideline for Practical Salinity formula also covering the low salinity range.

15.2 Discussion on Supplementary Release for a simplified density equation for oceanographic use.

15.3 Appointment of Task Groups, if appropriate.

16. Reports on miscellaneous TPWS scientific topics (joint with WG IRS)

16.1 Thermophysical property research at Helmut-Schmidt-University in Hamburg (K. Meier)

16.2 A comparative study of $P_s(T)$ models for H_2O in the critical region (E. E. Ustyuzhanin, V. F. Ochkov)

16.3 Online calculation from IAPWS formulations (V. Ochkov, K. Orlov)

16.4 Innovative concept for fluid property approximations (M. Hiegemann)

17. Joint session with WG PCAS [Thursday morning]
    - 17.1 Report of Task Group on Transport Properties of Seawater, joint with SC SW and WG IRS (A. Anderko, A. Harvey)
    - 17.2 Report of Evaluation Task Group for Seawater Thermal Conductivity (R. Pawlowicz)
    - 17.3 Formal consideration of Guideline on Thermal Conductivity of Seawater
    - 17.4 Progress toward improved ideal-gas properties of ordinary and heavy water (J. Hrubý)
    - 17.5 Development of first-principles data to extend knowledge of the second virial coefficient of ordinary and heavy water (A. Harvey, G. Garberoglio, P. Jankowski, K. Szalewicz)
    - 17.6 Modeling thermodynamic properties of mixtures of natural substances used as working fluids for heat pumps and organic Rankine cycle (H. Miyamoto, R. Akasaka, E. Lemmon)
18. IAPWS Certified Research Needs (ICRNs)
    - 18.1 ICRN 27: Thermophysical Properties of Humid Gases and CO_2-Rich Mixtures (closing statement needed) (R. Span, A. Harvey)
    - 18.2 ICRN24: Thermal conductivity of water vapor
19. Reports on other TPWS activities
    - 19.1 Guideline on Fundamental Constants (A. Harvey)
    - 19.2 Advisory Note 2 (J. Cooper, A. Harvey)
20. Other Business
    - 20.1 Report on International Collaborative Projects
    - 20.2 Discussion of IAPWS document numbering/designation
    - 20.3 Topics for 2018 ICPWS
21. Membership
22. Contribution to Press Release
23. Preparation of the Formal Motion to the EC
24. Adjournment