IAPWS Thermophysical Properties of Water and Steam WG
Turin, Italy, 3-8 September 2023

NOTE: These Minutes include some items that were held jointly with the IRS and/or PCAS Working Groups. 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, September 4 at approximately 10:30 by the TPWS Chair, Karsten Meier. TPWS Agenda was adopted (Attachment A). The 2022 Minutes had been circulated and approved by email shortly after the 2022 meeting. Jan Hrubý was appointed Clerk of Minutes for TPWS.

3. Potential International Collaborative Projects. No new project was suggested.

4. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95)

4.1 Report of Task Group (A. Harvey, D. Friend, J. Hrubý, N. Okita, R. Span)
Relevant ICRN 31 was adopted in 2019. A. Harvey reviewed the performance of IAPWS-95 with new existing data, starting needs of new data. Places for improvement: obsolete gas constant, problematic terms to mimic critical behavior, extrapolation to supercooled water. Oscillations in $p(\rho)$ inside the binodal can distort mixture calculations and prohibit using in models of vapor-liquid phase interface. Fourth virial coefficient is unphysically large. In a discussion, it was suggested an option to develop an auxiliary equation valid in a neighborhood of the vapor-liquid critical point. R. Span mentioned that the accurate scaling behavior is not much important for application in technology, because at process conditions equilibrium is hardly established at near-critical conditions. K. Meier mentioned that new data from his laboratory is available for the speed of sound in liquid water in an extended temperature range. A. Harvey indicated that experimental results which will be used in the new equation should be available roughly within 5 years. R. Span stated that this allows only experiments with existing experimental facilities. **The task group was extended by S. Lago (as a vicechair), A. Giuliano Albo and Y. Kayukawa** to motivate experimental work **and by F. Caupin** to cover the metastable water region.

5. IAPWS Certified Research Needs (ICRNs)
Decision about this ICRN 16 (Thermophysical Properties of Seawater) and ICRN 30 (Thermophysical Properties of Supercooled Water) was postponed to the 2024 meeting, where more seawater and supercooled water experts should be present.

6. Industrial Requirements and Solutions for Property Calculations (joint with WG IRS and SCSW) [Monday afternoon]
NOTE: Item 6 is reported on in the IRS Minutes.

6.1 Report on a white paper for acid gas dew points (N. Okita)

6.2 Report of the Task Group "Categories of industrial requirements" (N. Okita, chairs or representatives of other WG)

6.3 Discussion on how to best exploit the work carried on last year by IRS WG (concerning industrial requirements)

6.4 Report of the Task Group "Wet steam properties calculation" (A. Nový, J. Hrubý, R. Span, K. Meier, F. di Mare, S. Senoo, M. Kunick)

6.5 Translation of IF-97 Fortran routines into other programming languages (A. Nový)

7. 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, R. Mareš, F. Caupin)
J. Hrubý reported that the persisting problem is lack of experimental data at high temperatures (roughly above 100°C). Possibility of obtaining new data in this region is being evaluated. At present, it is possible to revise the uncertainties stated in R1-76(2014). With respect to present data, it is apparent that the uncertainties can be substantially reduced for the near-ambient temperature range.

8. Heavy Water Properties (joint with WG IRS)

8.1 Thermodynamic property measurements for heavy water at metastable states (Y. Kayukawa, H. Miyamoto, and R. Akasaka) For computations of thermodynamic properties of mixtures using contemporary models, the properties of pure water are often needed at conditions of metastable liquid. To provide data for improving the equations of state in these regions, density and speed of sound measurements are developed for heavy water. In the discussion, it was pointed out that such experimental data would be needed for ordinary water, however with uncertainties comparable with those in the stable region.

8.2 Progress on a formulation for the static dielectric constant of heavy water (J. Cox, A. Harvey, and P. Tremaine) The formulation is to be developed in two steps. In the first step, correlation for liquid heavy water valid in a limited temperature range will be developed. In a second step, correlation for the full range of parameters will be developed.

9. Reports on miscellaneous TPWS scientific topics (joint with IRS and PCAS)

9.1 Multimodal CO_2-transport - Current developments, the relevance of thermodynamic properties and open questions regarding the formation of corrosive phases (R. Span)
Recently, establishing CO2 pipelines in Germany is considered, with storage sites in Norway, Netherlands, or UK. Possible EU development of CO2 pipeline

backbone (parallel to the H2 backbone) to connect states with limited approach to suitable storage locations. There is a need to balance costs of cleaning with costs of pipe material, which requires better knowledge of the behavior of CO2 rich mixtures. Combination o pipeline with ship transport is considered (compressed gas in pipes, dense phase in ships). Standards for CO2 compositions (H2O, H2S, CO, O2, SOx, NOx) are being developed. Expert Group of the CCUS-Forum outlined fundamentals for standards. Two phase flow should be avoided as much as possible. Formation of corrosive phases must be avoided. Health and safety impact of impurities should be smaller than that of CO2 itself. Negotiable (such as N2 and Ar non-condensables) and non-negotiable impurities (primarily due to health and safety) are distinguished. Instead of specifying detailed composition of non-condensable gases, it is possible to define a minimum boiling temperature for a given pressure. SOx problem – usually SOx is measured, but SO3 reduces the dew point much stronger than SO2.

10. Joint session with WG PCAS [Tuesday morning]

10.1 Cross second and third virial coefficients and dilute-gas transport properties of the water–argon system from first-principles calculations (R. Hellmann)
New H2O-Ar and non-additive H2O-Ar-Ar potential energy surfaces based on ab initio calculations were developed. The computed data was fitted to analytical functions of temperature. The results for the cross-second virial coefficient are in good agreement with earlier computations by Hodges et al. (2002). Experimental data for virial coefficient and Joule-Thomson coefficient show much higher uncertainties. Shear viscosity and thermal conductivity depend on composition non-linearly even in the zero-density limit. In the discussion, it was pointed out that, for practical applications, H2O-Ar-Ar is much more important than H2O-H2O-Ar (which was not computed). The reason is that water is usually very dilute and the corresponding ternary interactions are statistically unimportant.

10.2 Report of the Task Group on the enhancement factor of mixtures containing steam (K. Meier, R. Hellmann, A. Harvey, and V. Fernicola). Goal is an IAPWS guideline providing enhancement factors for solubility of water vapor in important gases at elevated pressures. As a pilot project, one system (presumably water-argon) will be chosen.

10.3 A new model for thermodynamic properties of mixtures based on Helmholtz energy formulations of the components yielding a proper composition dependence of virial coefficients. Preliminary results for water-gas systems. (J. Hrubý)
Contemporary corresponding states-based method of modeling fluid mixtures with multi-component equations of state generates unphysical composition dependence of virial coefficients. The suggested model overcomes this problem. Predictive capabilities of the model were demonstrated with methane-propane system. Cross-second virial coefficients for water-gas systems (Ar, N2, H2) can be reproduced when a few model parameters are fitted. To be usable for the

presented mixture model, the equations of state of pure components (in particular for water) must extrapolate well into the metastable region.

10.4 A Calibration facility for investigating trace water sensors in moist hydrogen in a wide range of gas pressure and water concentration (R. Nobakht, R. Cuccaro, R. Salerno, and V. Fernicola).
Sensors like capacitance aluminum oxide, quartz crystal microbalance, infrared spectroscopy are affected by hydrogen. A transportable precision humidity generator was developed. Enhancement factor needs to be known for the calibration procedure. An experimental set up allowing to measure the enhancement factor in flow configuration is being developed. The measuring procedure, involving expansion to lower pressure reducing the non-ideal effects, was discussed.

10.5 Measurements of the surface tension of the binary mixtures water + ethylene glycol and water + methanol at temperatures down to -25 °C (V. Vinš, M. Součková, M. Čenský, O. Prokopová, A. Blahut and J. Hrubý)
Experimental set up originally developed for measurement of surface tension of pure water at conditions of supercooled liquid were used to study selected aqueous solutions. Three variants of the capillary rise method were implemented. Evaluation of the surface tension requires knowledge of density, which was measured as function of temperature and composition using a vibrating tube densimeter. A correlation for the density of aqueous ethylene glycol was developed. At present, experiments focus on the surface tension for aqueous solutions of salts.

11. Reports on seawater-related topics (joint with SC SW) [Tuesday afternoon]

11.1 Present status of the absolute density measurements for sea-water (Y. Kayukawa)
The goal of the development is improving the uncertainty of the equation of state to ppm level. Use is made of a silicon single crystal sphere and sinker manufactured for the purpose of kilogram re-definition. Hydrostatic weighing apparatus for seawater density was developed. The weighing mechanism is enclosed in a pressure-controlled containment to avoid effect of atmospheric pressure fluctuation. Yet some relation of the evaluated densities to atmospheric pressure was observed.

11.2 How (sea) water cooling water systems can remove nano- and micro-plastics from our marine environment (L. Daal).
Nano- and micro-plastics are environmental pollutants receiving considerable attention in recent years. The water treatment facilities of existing powerplants can be used to remove plastics particles. Promising results of the cleaning process were presented.

11.3 Discussion on the future of the TEOS-10 equation: management and updating
At present, TEOS10 continues to be maintained by Joint Committee on Seawater (JCS). Further discussion is postponed to the 2024 meeting.

11.4 Discussion on the future of the Subcommittee on Sea Water (SCCW).
S. Seitz wrote a Distress Flyer on the situation in SCCW and distributed it to potentially interested public. Four positive responses were received. D. Friend suggested that presentations on seawater topics at 18th ICPWS could encourage the activity. A. Giuliano Albo agreed to co-chair a conference session on sea water. S. Seitz agreed to assist.

12. Joint session with WG PCAS
NOTE: Item 12 is reported in PCAS minutes.

12.1 Revaluation of the database and formulation for the water ionization constant (K_w) (H. Arcis)

TPWS session [Thursday morning]

13. IAPWS Webpage
IAPWS webpage was discussed. The present appearance is obsolete and more contents should be included, in particular description of TPWS aims and activities. **K. Meier will prepare a short document concerning the contents of webpage needed for TPWS.**

14. Discussion on the future activities of TPWS
14.1 Active TPWS Task Groups were reviewed: Development of a New Formulation for the Thermodynamic Properties of Ordinary Water, Surface Tension of Ordinary Water, Enhancement Factor of Mixtures Containing Steam, Formulation for the Static Dielectric Constant of Heavy Water, Diffusivity of Ordinary Water, Possible Revision of IAPWS Formulations for Melting Curves. TPWS Chair is requested to contact the chairs of the TG and ask them for presentations of their outputs at 18th ICPWS.

14.2 Possible future areas of interest to TPWS: equation of state for ordinary water in the critical region, thermophysical properties of water-based heat transfer fluids, new formulation for ammonia-water, properties of geophysical fluids, radiation chemistry, equilibrium constants of reactions in aqueous solutions (particularly for power plant application).

15. Report on International Collaborative Projects.
The TPWS Chair requested the group to remind the members of the possibility of establishing international collaborative projects.

16. Membership. There were no changes in TPWS membership.

17. Contribution to Press Release
The Chair and Clerk of Minutes were assigned to prepare the contribution to the Press Release.

18. 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.

19. Adjournment
    The meeting was adjourned at approximately 11:00 on Thursday, September 7.

Agenda for the IAPWS Working Group
Thermophysical Properties of Water and Steam (TPWS)
Turin, Italy, Sept. 3 – Sept. 8, 2023

1. Opening Remarks; Adoption of Agenda [Monday morning, joint with WG IRS and SCSW]
2. Appointment of Clerk of Minutes
3. Potential International Collaborative Projects
4. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95)
   - 4.1 Report of Task Group (A. Harvey, D. Friend, J. Hrubý, N. Okita, R. Span)
5. IAPWS Certified Research Needs (ICRNs)
   - 5.1 ICRN 16: Thermophysical Properties of Seawater (R. Pawlowicz)
   - 5.2 ICRN 30: Thermophysical Properties of Supercooled Water (O. Hellmuth)
6. Industrial Requirements and Solutions for Property Calculations (joint with WG IRS and SCSW) [Monday afternoon]
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TPWS session [Thursday morning]

13. IAPWS Webpage
14. Discussion on Future Activities of TPWS
    14.1 Review of current TPWS task groups
    14.2 Possible future areas of interest to TPWS
15. Report on International Collaborative Projects
16. Membership
17. Contribution to Press Release
18. Preparation of the Formal Motion to the EC
19. Adjournement

September 4, 2023

K. Meier (Chair), J. Hrubý (Vice-Chair)