IAPWS Thermophysical Properties of Water and Steam WG
Rotorua, New Zealand, 28-29 November 2022

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, November 28, 2022, at approximately 10:30 by the TPWS Chair, Karsten Meier. A modified Agenda was adopted (Attachment A). The 2021 Minutes had been circulated and approved by email shortly after the 2021 virtual meeting. Allan Harvey was appointed Clerk of Minutes for TPWS.

3. Tributes for deceased colleagues.

A. Harvey presented brief tributes to three IAPWS contributors who had died in recent years: Bob Spencer (IAPWS Honorary Fellow), Bill Parry, and Christopher Wormald. H.-J. Kretzschmar read a tribute to Francisco (Pancho) Blangetti that had been prepared by Michael Hiegemann and Bobby Swoboda. The Chair led the Working Groups in a moment of silence.

4. Potential International Collaborative Projects

The Working Group discussed a proposed project (involving the Czech Republic, Germany, and the U.S.) titled "Towards a replacement for the IAPWS Formulation 1995: Detailed analysis of available data". **The WG unanimously endorsed the proposal**.

5. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95). (A. Harvey, D. Friend, J. Hrubý, N. Okita, K. Orlov, R. Span)

A. Harvey reported on the various reasons for replacing IAPWS-95 in the coming years (including small flaws in the equation of state, new data including many good sound-speed measurements, advances in technology for developing reference equations of state). There are still some data needs as expressed in IAPWS ICRN 31, but it seems unlikely that many of these needs will be met in the timeframe envisioned for the effort. A question was raised about when a new EOS might be ready, but it is too early to say. It was discussed that the new EOS should behave accurately for the metastable vapor and liquid below the triple point, and that more rigorous uncertainty information would be desirable.

6. Metrology for trace water in ultra-pure process gases (P. Alberto Giuliano Albo)

P.A. Giuliano Albo reported on the PROMET-H2O project led by his colleague Vito Fernicola. The purpose is to develop metrology for measurement of trace amounts of water in ultra-pure process gases in applications including energy systems and semiconductor processing. Pressures will be up to 1 MPa, with dew-point temperatures ranging from −105 °C to −65 °C corresponding to roughly 5 ppb to 5 ppm H_2O in the gas. Several different experimental approaches are being explored, and there will be some component of developing recommended enhancement factors for ice in common gases. It was discussed that those recommendations might be made into an IAPWS Guideline (see item 11.2).

7. IAPWS Certified Research Needs (ICRNs)

Two expired ICRNs were discussed, although in neither case were the key people present. For ICRN-16 (Properties of Seawater), **J. Hruby and R. Pawlowicz (if the latter is willing) were appointed as a Task Group to evaluate the situation and bring a recommendation to the 2023 meeting**. For ICRN-30 (Properties of Supercooled Water), some new data have become available but a new leader of the IAPWS efforts in that area is needed as O. Hellmuth is not able to continue. **The WG Chair will contact F. Caupin about taking the lead in revising the ICRN**. If that is not possible, we will discuss in 2023 how to proceed, perhaps by making a Closing Statement.

NOTE: Item 8 is reported on in the IRS minutes.

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

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

9. Heavy Water Properties

9.1 Progress on a formulation for the static dielectric constant of heavy water (J. Cox, J. Young, A. Harvey, and P. Tremaine)

A. Harvey reported on behalf of the Task Group, which has been slowed by the departure of J. Young from NIST. Work is expected to resume in early 2023. The plan is to make one formulation that would be a simple modification or correction to the IAPWS H_2O formulation, limited to the liquid up to perhaps 300 °C, and then a second, comprehensive formulation covering the whole fluid range that would not have the flaws of the H_2O formulation. The time frame is still unclear due to limited availability of personnel. It was recalled that in 2021 we authorized the WG Chair to appoint an Evaluation Task Group during the year if it was warranted.

10. Report of Task Group on surface tension of ordinary water (joint with WG IRS and SC SW) (J. Kalová, V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, R. Mareš, F. Caupin)

J. Hrubý reported that a new correlation had been published in the past year by Kalová and Mareš. In the discussion, the consensus was that, in the absence of new data (particularly at high temperatures), there was no clear reason to produce a new formulation for IAPWS. However, at some temperatures the uncertainty estimates in the IAPWS formulation are too large, so a revision of those estimates could be worthwhile.

11. Joint session with WG PCAS

11.1 Crystal growth of urea and its modulation by additives as analyzed by all-atom MD simulation and free-energy calculation (N. Matubayasi)

This was a technical presentation about insights gained by molecular simulation on the relative growth rates of different crystal planes in urea.

11.2 Cross second virial coefficients for binary mixtures of water vapor with carbon monoxide, sulfur dioxide, hydrogen sulfide, and hydrogen from ab initio intermolecular potentials (R. Hellmann, K. Meier)

K. Meier reported on the project of calculating high-quality second virial coefficients for water-gas systems based on state-of-the-art ab initio pair potentials. Future calculations will involve water with argon and the light alkanes. These can contribute to calculation of enhancement factors in various contexts.

In subsequent discussion, it was noted that this has overlap with the enhancement factor needs of the PROMET-H2O project discussed in item 6. An IAPWS Guideline on values of $B_{12}(T)$ and/or on the enhancement factor of water and ice in common gases would be useful for a variety of purposes. **A Task Group was appointed consisting of K. Meier, R. Hellmann, A. Harvey, and V. Fernicola (if he is willing to join), with the mission to decide what makes the most sense for a Guideline and to work toward preparing recommended values in convenient form.**

11.3 (This item was cancelled).

11.4 Challenges in modeling the ammonia/water system (I. Bell, A. Harvey)

A. Harvey, on behalf of his colleague Ian Bell, presented some of the problems with the present IAPWS model for the thermodynamics of ammonia/water, along with the data situation for sound speed where the sets of data seem to not be mutually consistent. Some high-quality liquid sound speeds, even if only near atmospheric pressure, would be very helpful in sorting out the proper behaviour. Several factors making this mixture difficult to study were discussed.

12. Reports on seawater-related topics

12.1 New accurate data for the density of cold and supercooled seawater at practical salinity 35 and pressures up to 110 MPa (A. Blahut, J. Hrubý, V. Vinš)

J. Hrubý presented his group's measurements of seawater density extending to 100 MPa and about 10 K of supercooling below the freezing curve. Compared to the IAPWS seawater formulation, there are some significant differences in thermal expansivity in the supercooled region and to some extent along the melting curve.

12.2 A new approach to a comprehensive formulation of thermodynamic properties of seawater (J. Hrubý, A. Blahut)

J. Hrubý reported a new approach to seawater thermodynamics his group has taken involving scaling the pure-water equation and adding an extended Debye-Hückel term. The maximum density points are used in the scaling from the IAPWS supercooled water guideline. Initial results seem promising.

12.3 Discussion on future of Subcommittee on Seawater

The absence of our seawater contingent from this meeting, and from IAPWS in the past 2 years or so, was noted. An email had been received from SCSW Chair Rich Pawlowicz about his difficulty in participating and wondering if the Subcommittee

should be folded back into the TPWS Working Group. The Joint Committee on Seawater is still somewhat active with Pawlowicz as Chair and Steffen Seitz of PTB as a Vice-Chair, but its current work is less IAPWS-related. **It was recommended that the SCSW remain as it is in IAPWS for now, with the following steps to be taken to attempt to revive it: K. Meier contact Pawlowicz, Feistel, and Seitz to get their input on a way forward. P.A. Giuliano Albo contact people he knows in physical oceanography in Italy and France to invite them to the 2023 IAPWS meeting.**

13. TPWS/IRS/PCAS/PCC joint session

This item is reported in the PCC Minutes.

15. Membership

Michal Duška (Czech Republic) was unanimously elected as a new TPWS member.

16. Election of Vice-Chair

A. Harvey will step down as Vice-Chair after the conclusion of this meeting. K. Meier remains as Chair and J. Hrubý remains as Vice-Chair.

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 17:00 on Tuesday, November 29.

Agenda for the IAPWS Working Group

Thermophysical Properties of Water and Steam (TPWS)
Rotorua, New Zealand, Nov. 27 – Dec. 2, 2022

1. Opening Remarks; Adoption of Agenda [Monday morning]
2. Appointment of Clerk of Minutes
3. Minute's Silence for Deceased Members and Colleagues (A. Harvey, H.-J. Kretzschmar)
4. Potential International Collaborative Projects
5. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95)
   - 5.1 Report of Task Group (A. Harvey, D. Friend, J. Hrubý, N. Okita, K. Orlov, R. Span)
6. Reports on miscellaneous TPWS scientific topics
   - 6.1 Metrology for trace water in ultra-pure process gasses (P. Alberto Giuliano Albo)
7. IAPWS Certified Research Needs (ICRNs)
   - 7.1 ICRN 16: Thermophysical Properties of Seawater (R. Pawlowicz)
   - 7.2 ICRN 30: Thermophysical Properties of Supercooled Water (O. Hellmuth)
8. Industrial Requirements and Solutions for Property Calculations (joint with WG IRS) [Monday afternoon]
   - 8.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, chairs or representatives of other WG)
   - 8.2 Report of the Task Group "Wet steam properties calculation" (A. Nový, J. Hrubý, K. Orlov, R. Span, K. Meier, Francesca di Mare, S. Senoo, M. Kunick)
9. Heavy Water Properties (joint with WG IRS)
   - 9.1 Progress on a formulation for the static dielectric constant of heavy water (J. Cox, J. Young, A. Harvey, and P. Tremaine)
   - 9.2 Appointment of a Task Group for the evaluation of the formulation of the static dielectric constant of heavy water
10. Report of Task Group on surface tension of ordinary water (joint with WG IRS and SC SW) (J. Kalová, V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, R. Mareš, F. Caupin)
11. Joint session with WG PCAS [Tuesday morning]
    - 11.1 Crystal growth of urea and its modulation by additives as analyzed by all-atom MD simulation and free-energy calculation (N. Matubayasi)
    - 11.2 Cross second virial coefficients for binary mixtures of water vapor with carbon monoxide, sulfur dioxide, hydrogen sulfide, and hydrogen from *ab initio* intermolecular potentials (R. Hellmann, K. Meier)
    - 11.3 Speed of sound measurements in mixtures of ammonia and water (M. Brown, A. Harvey)

11.4 Challenges in modeling the ammonia/water system (I. Bell, A. Harvey)

12. Reports on seawater-related topics (joint with WG PCAS and SC SW)
    12.1 New accurate data for the density of cold and supercooled seawater at practical salinity 35 and pressures up to 110 MPa (A. Blahut, J. Hrubý, V. Vinš)
    12.2 A new approach to a comprehensive formulation of thermodynamic properties of seawater (J. Hrubý, A. Blahut)
    12.3 Discussion on the future of the Subcommittee on Sea Water
13. TPWS/IRS/PCAS/PCC joint session [Tuesday afternoon]
    13.1 Electrode boiler chemistry issues update and possible TGD discussions (D. Addison, M. Nielson)
    13.2 ICRN 32 Conductivity of Electrolytes in Aqueous Solutions presentation and discussion
    13.3 Strategies to improve criteria on steam for steam turbine (geothermal) (S. Terada)
    13.4 Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, F. di Mare, D. Addison, S. Terada)
    13.5 Report of the Task Group "Wet steam data from operating turbines" (S. Senoo, N. Okita, A. Anderko)
    13.6 Report of the joint Task Group on ICRN for acid gas dew points (N. Okita, S. Senoo, T. Němec)

Tuesday afternoon session splits into separate WG sessions

14. Other Business
    14.1 Report on International Collaborative Projects
15. Membership
16. Election of Vice-Chair
17. Contribution to Press Release
18. Preparation of the Formal Motion to the EC

November 27, 2022

K. Meier (Chair), A.H. Harvey, J. Hrubý (Vice-Chairs)