

IAPWS Thermophysical Properties of Water and Steam WG Prague, Czech Republic, 2 September 2018

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 Sunday, September 2, 2018 by the TPWS Chair, Allan Harvey. The agenda (Attachment A) was adopted without additions. The Chair noted that the 2017 Minutes had been circulated and approved by email shortly after the 2017 meeting. K. Meier was appointed Clerk of Minutes for TPWS.

3. No new Collaborative Project was suggested at TPWS.

NOTE: Item 4 is reported on in the IRS minutes.

4. Industrial Requirements and Solutions for Steam Property Calculations (joint with WG IRS)

4.1 Report of the Task Group “Categories of industrial requirements”

4.2 Report of the Task Group “Industrial Advisory Note”

4.3 Report of the Task Group “Wet steam properties calculation”

4.4 Report of the Task Group “Wet Steam Data from Operating Turbines”

5. Minor Revisions to IAPWS Documents (joint with WG IRS)

5.1 Report on minor revision of IAPWS-95 Release (A. Harvey)

A. Harvey reported on the revision of the release on behalf of the Task Group. Additional explicit equations for the second virial coefficient $B(T)$ and third virial coefficient $C(T)$ obtained analytically from the IAPWS formulation were added. Furthermore, sentences were added to the captions of the figures for uncertainty stating that the uncertainties of the density, heat capacities, and speed of sound in the gas phase become much smaller at low pressures as the ideal gas limit is approached.

5.2 Report on evaluation of IAPWS-95 revision (K. Miyagawa, presented by A. Harvey)

A. Harvey presented the evaluation report on the Revised Release on behalf of K. Miyagawa. K. Miyagawa verified the equations for the virial coefficients, and recommends to accept the Revised Release. It was discussed whether a sentence should be added to the footnote in the list of symbols stating that the change to the new SI unit system in 2019 will have no impact on the formulation. It was decided to add such a note. The wording should be agreed upon by the Chair and the Vice-chairs. After the meeting, R. Span, S. Bell, and D. Friend were also included in this

decision and the sentence “This is unaffected by the revision to the SI system of units scheduled to go into effect in 2019.” was agreed upon.

5.3 Formal consideration of IAPWS-95 Revised Release

The WG voted to approve the revised Release and recommend that the EC send it for approval by Postal Ballot.

5.4 Report on minor revision of Advisory Note 3 on Thermodynamic Derivatives from IAPWS Formulations (H.-J. Kretzschmar)

H.-J. Kretzschmar presented the revision of the advisory note. The note provides equations for derivatives of the IAPWS Formulations for ordinary water, heavy water, and seawater, which are formulated as fundamental equations in terms of the Helmholtz or Gibbs energies. The note is intended to assist implementation of the IAPWS Formulations. The update became necessary because of the 2018 Release of the new IAPWS Formulation for heavy water.

5.5 Report on evaluation of Revised Advisory Note 3 (K. Meier)

K. Meier reported on behalf of the Task Group about the Evaluation of the Revised Note. All revised equations were verified. Minor editorial changes were suggested. The equations in the Revised Note were provided in specific quantities whereas the equations in the IAPWS Release are given in molar quantities. To remove this inconsistency the calculated quantities are retained as specific quantities, while the molar density was replaced by the product of molar density and molar mass and the molar gas constant by the ratio of the universal gas constant to the molar mass in all equations for the heavy water formulation. This change resulted in a twofold use of the symbol R , for the universal gas constant in the equations for the heavy water formulation and for the specific gas constant in the equations of all other formulations. This ambiguity is acceptable. K. Meier recommends to approve the Revised Note by IAPWS.

5.6 Formal consideration of Revised Advisory Note 3

The WG voted to approve the revised Release and recommend that the EC send it for Postal Ballot following review by the Editorial Committee.

6. Heavy Water Properties (joint with WG IRS)

6.1 Report of Task Group on Heavy Water Thermodynamic Properties (R. Span, A. Harvey, S. Herrig)

S. Herrig reported on behalf of the Task Group on a revision of the Release of the IAPWS formulation for heavy water. An equation of state was presented at the 2017 Meeting in Kyoto, and the corresponding release became available online in 2018. During the publication process a further density data set (Kell, 1985) was found.

Since this density data set is more accurate than those to which the equation of state was fitted, it was decided to refit the equation. The fit resulted in a better representation of the Kell density data set and reduced uncertainties in the liquid phase density and a minor improvement in the uncertainties of the heat capacities and the speed of sound. Moreover, the saturated liquid density is represented much better, and the critical pressure is fitted within the uncertainty specified by IAPWS. The IAPWS release was updated for these points. A manuscript reporting the refitted equation of state has been submitted to the Journal of Physical and Chemical Reference Data.

6.2 Report of Evaluation Task Group for Revised Heavy Water Formulation (H.-J. Kretzschmar)

H.-J. Kretzschmar reported on behalf of the Task Group on the evaluation of the Revised Release. The revision resulted only in minor changes of the release. Especially the equations, the tables for the coefficients and figures for uncertainty were revised. The draft contains all required information. All equations were programmed and computationally verified. The document contains all necessary background information and relevant references. It is of excellent quality. H.-J. Kretzschmar recommends to adopt the revised Release by IAPWS. At the suggestion of D. Friend, a note will be added like that described in item 5.2 above.

6.3 Formal consideration of Revised Release for Heavy Water

The WG voted to approve the revised Release and recommend to the EC that it be sent for Postal Ballot following review by the Editorial Committee.

6.4 Report of TG for Heavy Water Transport Properties (J. Sengers, M. Assael, M. Huber, R. Perkins)

A. Harvey reported the status of the work on behalf of the Task Group. Available data in the literature for the viscosity of heavy water have been collected and were evaluated. Four new data sets have been published since the Release of the IAPWS 1984 formulation. F. Caupin measured the viscosity of subcooled heavy water at ambient pressure and has provided the data to the Task Group. The new formulation will be formulated as a product of the zero-density viscosity, the residual contribution, and the critical enhancement. The zero-density viscosity is based on the theoretical data of Hellmann and Bich and formulated as a ratio of two polynomials in temperature. The residual and critical enhancement contributions will be developed before the 2019 IAPWS Meeting in Banff. R. Hellmann remarked that the functional form chosen for the zero-density term does not represent the current state-of-the-art. It was recommended by the chairman that the Task Group should consult Robert Hellmann about how to fit the theoretical zero-density data in the best way.

7. 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, J. Pátek, F. Caupin)

J. Kalová reported on the surface tension of ordinary water. She recalled the history of the surface tension of ordinary water in IAPWS. The IAPWS formulation is valid since 1975. Several new data sets have been published since then. With the introduction of the ITS-90 in 1990 the value of the critical temperature changed. The IAPWS formulation and the Pátek et al. correlation are lower than the IAPWS comparison formulation. A new fit to experimental data is required. A revised IAPWS Guideline should also include reference values at 20 °C and 25 °C.

R. Mareš reported on new measurements of the surface tension of supercooled water in the temperature range between –19.4 °C and –32 °C with a vertical capillary tube technique. The new measurements extend the range of previous measurements, which cover the range from +2 °C to –25 °C, down to –32 °C. The dependence of the surface tension of supercooled water on temperature is almost linear.

8. Metastable Water (joint with SC SW)

8.1 Report on the vapor pressure of supercooled water (V. Holten, A. Harvey)

A. Harvey reported that there are several correlations for the vapor pressure of supercooled water, most of which are extrapolated outside their valid range, and described different approaches to calculate the vapor pressure (correlations as a function of temperature and from thermodynamic potentials). A thermodynamic potential for supercooled water in terms of the Helmholtz energy was developed by Holten et al. (2014). Vapor pressures calculated with IAPWS-95 and the EOS of Holten et al. agree within 0.01%. Deviations are higher at low temperatures. There are two data sets for the isobaric heat capacity for supercooled water that are not consistent. This inconsistency has an influence on the uncertainty of the vapor pressure calculated with the equation of state. A. Harvey recommends to use the Holten et al. equation of state for vapor pressure calculation and to add the calculation of the vapor pressure to the IAPWS Guideline on the Thermophysical Properties of Supercooled Water. The uncertainty of the vapor pressure should be based on the uncertainty of the isobaric heat capacity. The draft revision of the Guideline should be circulated in time for adoption at the 2019 meeting in Banff.

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

A. Harvey reported on a possible revision of the IAPWS formulations for melting curves. The triple point for liquid water/ice I/ice III is not described accurately and this issue should be improved. There is no clear plan at this time for improving the formulation due to the unavailability of V. Holten to work on it.

NOTE: Items 9 and 10 are reported on in the SC SW minutes.

9. Cooperation with other international bodies (joint with SC SW)

- 9.1 IAPWS/IAPSO/SCOR Joint Committee on Seawater, including updates to TEOS-10
- 9.2 BIPM/IAPWS cooperation

10. Proposed new IAPWS seawater-related documents (joint with SC SW)

- 10.1 Report on surface tension of seawater
- 10.2 Appointment of Evaluation Task Group for seawater surface tension and setting of schedule for new IAPWS Guideline
- 10.3 Report on preliminary work on viscosity of seawater

11. IAPWS Certified Research Needs (ICRNs)

- 11.1 ICRN 27: Thermophysical Properties of Humid Gases and CO₂-Rich Mixtures (closing statement needed) (R. Span, A. Harvey)

A. Harvey reported that the closing statement will be prepared soon; R. Span has just completed a first draft.

- 11.2 Report of Task Group on ICRN for acid gas dew points (N. Okita, K. Orlov, R. Span)

N. Okita reported on behalf of the Task Group on the status of the preparation of the ICRN. Different methods for dew point estimation were evaluated. It seems that the Abel function from 1946 is often used. It is the final goal to provide a recommendation for dew point estimation. Possibly the development of an estimation method can be supported by molecular simulations and/or simulations with ASPEN. A first draft of the ICRN will be presented at the 2019 meeting in Banff.

12. Reports on other TPWS activities

- 12.1 Guideline on Fundamental Constants (A. Harvey)

A. Harvey reported that there are no changes needing an update of the Guideline on Fundamental Constants.

- 12.2 Advisory Note 2 (J. Cooper, A. Harvey)

The Task Group was authorized to update this document to reflect the minor revisions to the IAPWS-95 Release.

- 12.3 Report on progress toward IAPWS Guideline on diffusivity of ordinary water (A. Harvey, K. Yoshida)

A. Harvey reported on behalf of the Task Group the status of the development of a correlation for the diffusivity of ordinary water. K. Yoshida measured the self-diffusion coefficient at high temperatures and published a correlation. The

correlation yields unphysical behavior in the zero-density limit when extrapolated to low temperature, where the calculated self-diffusion coefficient becomes negative. Therefore, it was decided to develop a new correlation. The zero-density contribution was fitted by M. Huber (NIST, Boulder) to the theoretical data of Hellmann and co-workers. Next steps are the collection and evaluation of experimental data and fitting of the residual part. The self-diffusion coefficient does not have a critical anomaly as the viscosity and thermal conductivity. Finally, the correlation will be published and established as an IAPWS formulation in a Guideline. **A. Harvey suggested to add M. Huber as an external expert and R. Hellmann to the Task Group; in subsequent discussions F. Caupin was also added to the Task Group. K. Meier resigned from the Task Group. An Evaluation Task Group (K. Meier, K. Orlov) was appointed (with possible additional membership from PCAS). The new members of Task Group and the Evaluation Task Group were unanimously approved.**

13. Other Business

It was discussed how the ICPWS conference series should be continued. R. Span pointed out that it is difficult to find funding for the research topics of interest to TPWS. He suggested to join the conference with other conferences or let it die and concentrate on the annual meetings. It was decided to postpone the discussion to the 2019 meeting in Banff and put the topic on the agenda for all working groups.

14. Membership

Dr. Robert Hellmann (University of Rostock, Germany) and Prof. Cornelia Breitkopf (Technical University Dresden, Germany) were unanimously elected as TPWS members. Henning Wolf (Germany) has retired and should be removed from TPWS membership.

15. Contribution to Press Release

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

16. 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.

17. Adjournment

The meeting was adjourned at 17:20 on Sunday, September 2.

**Agenda for the IAPWS Working Group
Thermophysical Properties of Water and Steam (TPWS)
Prague, Czech Republic, September 2, 2018**

1. Opening Remarks; Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Potential International Collaborative Projects
4. Industrial Requirements and Solutions for Steam Property Calculations (joint with WG IRS)
 - 4.1 Report of the Task Group “Categories of industrial requirements” (N. Okita, A. Nový, I. Weber)
 - 4.2 Report of the Task Group “Industrial Advisory Note” (M. Hiegemann, B. Rukes, A. Singh, A. Harvey) (N. Okita)
 - 4.3 Report of the Task Group “Wet steam properties Calculation” (A. Nový, J. Hrubý, K. Orlov, R. Span, K. Meier)
 - 4.4 Report of the Task Group “Wet Steam Data from Operating Turbines” (N. Okita, A. Nový, I. Weber, S. Senoo)
5. Minor Revisions to IAPWS Documents (joint with WG IRS)
 - 5.1 Report on minor revision of IAPWS-95 Release (A. Harvey)
 - 5.2 Report on evaluation of IAPWS-95 revision (K. Miyagawa, presented by A. Harvey)
 - 5.3 Formal consideration of IAPWS-95 Revised Release
 - 5.4 Report on minor revision of Advisory Note 3 on Thermodynamic Derivatives from IAPWS Formulations (H.-J. Kretzschmar)
 - 5.5 Report on evaluation of Revised Advisory Note 3 (K. Meier)
 - 5.6 Formal consideration of Revised Advisory Note 3
6. Heavy Water Properties (joint with WG IRS) [afternoon]
 - 6.1 Report of Task Group on Heavy Water Thermodynamic Properties (R. Span, A. Harvey, S. Herrig)
 - 6.2 Report of Evaluation Task Group for Revised Heavy Water Formulation (H.-J. Kretzschmar)
 - 6.3 Formal consideration of Revised Release for Heavy Water
 - 6.4 Report of TG for Heavy Water Transport Properties (J. Sengers, M. Assael, M. Huber, R. Perkins, presented by A. Harvey)
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