

Attachment 6

Minutes of the Working Group TPWS, 10-13 September 2001 as part of the IAPWS Annual Meeting, Gaithersburg, Maryland, USA.

After opening remarks from the WG Chairman Dr. D. Friend, the agenda included here as TPWS Attachment A was approved. Mr. J. Gallagher was appointed Clerk of Minutes for this meeting, and the Minutes of the TPWS WG meetings in Prague, Sep 2000, were approved.

Following this, an informal review of the status of Releases, Guidelines and other documents for which this WG is responsible was carried out.

In joint session with WG IC, we were presented a final version of the Supplementary Release on IAPWS-IF97 Backward Function $p(h,s)$, and a report of the Evaluation Task Group. For details of this, see the Minutes of WG IC. Also, see the Minutes of WG IC for details concerning the Progress Report of the Evaluation Task Group for the Guideline on Tabular Taylor Series Expansion (TTSE) Method and the Progress Report of the Task Group for the Development of IAPWS-IF97 Backward Equations in Region 3.

The WG TPWS meeting separately Tuesday discussed the following:

The Transport Properties Task Group (D. Friend, J. Sengers, A. Alexandrov) and M. Assael, Vogel of IUPAC, reported that a data paper had been published (JPCRD, 2000) and that a Viscosity Correlation for H_2O and D_2O was published by Alexandrov and Mateev. An Evaluation Task Group (R. Mares, O. Sifner) had been established, and evaluation criteria were discussed. D. Friend reviewed events in recent years. Mares presented a report by R. Mares and O. Sifner titled Temperature Conversion of the Coefficient of Thermal Conductivity to ITS-90.

Meeting Wed 8:30 AM at the hotel after the revision of the schedule due to the closing of Federal facilities, we proceeded with the joint TPWS/PCAS Workshop on Molecular Simulation, Igor Svishchev of Trent University, of the Task Group on Molecular Simulation as chair. Prof R. Wood could not make his presentation, as he had to return to Delaware. For details of this Workshop, see the minutes of WG PCAS.

Continuing with the TPWS Schedule, A. Harvey reported on a review of the situation concerning NaCl-Water Correlations. The following currently exist:

NaCl-Water Thermodynamics, at Low/Moderate Temperatures: D.G. Archer JPCRD 1992 - has thoroughly reviewed the data, correlated using the 1990 Hill EOS covering the liquid from 250 to 600 K, p to 100 MPa using a Modified Pitzer ion-interaction model. Room for improvements suggested include converting to ITS90, use of IAPWS standards for water thermodynamic properties and dielectric constant. There are new data in 2000, and IAPWS95 should be used instead of Hill.

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NaCl-Water Thermodynamics (High Temperatures) by Anderko and Pitzer. Dissociation was ignored. Temperatures greater than 573 K examined. The method used was perturbation theory based on dipolar hard spheres.

NaCl-Water Thermodynamics (Critical Region) - IAPWS Guideline for critical line adopted in 2000 based on Anisimov and Sengers - combines two curves to reproduce dip thought to be due to the nearness of the 3-phase region.

A. Anderko presented a preliminary report on the prediction of the behavior of dilute aqueous solutions containing NH_3 and CO_2 , allowing the calculation of vapor-liquid equilibrium and the compositions of the condensed phase. He uses an activity coefficient model, identifying all species - vapor, aqueous, neutral and ions. Simultaneous phase and chemical equilibrium calculations can be made. The pH for 3-component solutions can be calculated, based on high quality thermochemical data (with the exception of the carbamate ion). VLE for $\text{H}_2\text{O}-\text{NH}_3$ and $\text{H}_2\text{O}-\text{CO}_2$ is very well reproduced

J. Bellows reported on the need for a new formulation for Combustion Gases as requested in our meeting last year. He began with an introduction to the Brayton Combustion Cycle used in these turbines. The components of combustion gases are air, CO_2 , steam (below critical). He argued that the pure components are near enough to ideal gas, but not necessarily the mixtures. His recommendation: we do not need a new formulation for the volumetric properties of individual combustion gases, but further investigations of mixture properties are needed. The situation with respect to C_p is not clear. After discussion, it was suggested that knowledge of 2nd virial coefficients might be sufficient. Prof. Wagner will prepare an overview of non-linearity in these components for next year to help answer the question as to whether it is time for IAPWS to consider these problems.

D. Friend presented status of Ammonia-Water Guideline: The Evaluation Report has been presented, minor wording changes made, the draft sent for editorial review, a few more minor changes made, and proposed final version presented here. It is noted that Prof. Uematsu of Keio University has new experimental data and suggests that on the basis of this that uncertainties be increased in densities to 1% in liquid and 2% in vapor, and that Prof. Oguchi of the Evaluation Committee questions the values used for reference constants. We agree that changes in these values are insignificant, but more attention should be paid to our various reference values in the future so that they agree with current standards. Publications should clearly state which values used and they should be the standard value at the time the publication was prepared. We will recommend to the Executive Committee that the changes are minor enough that they can proceed with final approval without additional time being required.

The ICRN for Ammonia-Water properties is expiring this year and we discussed resubmission. It has been suggested that we include diffusion coefficients in the new one.

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We decide that the current ICRN should be allowed to expire and a new one including diffusion coefficients could be considered next year.

A. Harvey and R. Fernandez-Prini bring to our attention that a Monograph they are preparing on solubilities of gases in water could result in a guideline to be presented next year.

The Working Group TPWS, meeting separately, discussed the following:

On our liaison with IEC – J. Cooper reported that there was nothing new to report, and we decided to continue until next year.

Notes on monograph by F. Franks on Water (recently published) - He makes some statements concerning steam tables that indicate we could bring material to his attention that he might not be aware of. We ask J. Cooper to talk to his National Committee about contacting Prof. Franks informally and suggesting some changes if a future revision were to be published.

We have the final Technical Report from Abdulagatov, Magee and Aliev on experimental CvVTx measurements of H₂O-CH₃OH mixtures, a collaborative project sponsored by IAPWS. The final values of experimental data will be published in refereed literature.

In a joint meeting of the Working Groups TPWS and IC, Miyagawa presiding, the following were discussed:

On an ICRN for Metastable Steam properties: there are no experimental data on the vapor side. We would like to encourage measurements in this region. Rukes will evaluate the needs of industry in this region and consider an ICRN for experimental data for next year. We suspect that probably industry doesn't know that the properties predicted by formulations have no experimental data behind them. We will hope for a draft for next year. Prof Wagner suggests that flow measurements have been made, and can be used to test the current or future equations in this region.

Web-site issues: We discussed the possibility of a product called Software and Documentation be available from IAPWS (to include the TTSE discussed previously). We will recommend to the EC to consider that if computer code is an integral part of an IAPWS product it should be available on the web. Should the core code for IF97 (as on the disc distributed to the National Committees) be available on the Internet? This would require support, and IAPWS probably could not do this. We voted to this put on the web 17 yes, 2 no. We should note on the web that this is an integral part of the release, but IAPWS cannot offer support. Voting on the question "Should all source code of IAPWS releases and guidelines be on web?" this was rejected yes 5, no 7. J Sengers moves we consider distributing code on future products on a case by case basis. Agreed unanimously. A task group will work towards getting all tables from releases in

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distributable (perhaps .pdf) form. We recommend not making graphs and charts available electronically, as National Committees are responsible for this. Also, we recommend that copyright notices appear in two places - in the code, and on web before downloading. We recommend that the EC should require the following copyright notice to appear when downloading from web: (Copyright and liability disclaimer should appear on web page before downloading and written as a comment within the code itself):

Copyright 20xx by the International Association for the Properties of Water and Steam. Use of this product is allowed in all countries, provided that attribution is given to the International Association for the Properties of Water and Steam.

We recommend to the EC that they seek legal advice on wording so as to avoid liabilities. These are major policy issues to be recommended to the EC, so that we recommend to the EC that statutes be reviewed as to any modifications that might be needed.

On Future Tasks and Collaborations:

Computer Simulation Task Group: We ask I. Svishchev to formally assemble a group and TPWS, PCAS Chairman will submit membership suggestions to WGs and EC.

D₂O Task Group - we would table work except for temperature scale change. J Cooper will be added to task group. There have been two new papers on D₂O and H₂O-D₂O mixtures in the critical region published in last two years. No new experimental work known.

Fundamental Constants Guideline, by Allan Harvey, recommended for adoption to the EC.

TPWS Membership - Prof. R. Jacobsen is nominated to be a member of TPWS. Seconded, no objection, and will be recommended to the EC.

Also we hear that J. Yata of Japan, would like to resign. We will accept and will draft a letter expressing our appreciation for his work over the years.

New Business - We have been asked to consider any structural changes in organization that might be advisable - none are suggested at this time. No other new business.

Our Working Group meetings were adjourned Thursday at noon.

TPWS Attachment A

Agenda IAPWS Thermophysical Properties of Water and Steam WG

GAITHERSBURG, MARYLAND, USA 9-14 SEPTEMBER 2001

Monday 10 September

1. Opening Remarks; Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Approval of Minutes of TPWS WG in Prague, 2000
4. Review of status of releases and other documents
5. ¹Supplementary Release on IAPWS-IF97 Backward Function $p(h,s)$
 - (a) Report of the Evaluation Task Group
 - (b) Acceptance of the Supplementary Release
6. ¹Progress Report of the Evaluation Task Group for the Guideline on Tabular Taylor Series Expansion (TTSE) Method
7. ¹Progress Report of the Task Group for the Development of IAPWS-IF97 Backward Equations in Region 3

Tuesday 11 September

8. Reports on Various TPWS Activities
 - (a) Transport Properties: evaluation & progress report
 - (b) D2O Thermodynamics
 - (c) Fundamental Constants
 - (d) Liaison with IEC
 - (e) Discussion concerning Felix Franks' monograph
9. ¹Topics on the Calculation of the Functions $p(h,s)$ and $T(h,s)$ using IAPWS-IF97 Basic and Backward equations
10. ¹Uncertainties in IAPWS-IF97
11. ²Workshop on Molecular Modeling
12. Additional presentations of interest to TPWS members
 - (a) ²H₂O plus NaCl mixtures
 - (b) ²H₂O plus CO₂: T, P, pH
13. ²Ammonia-water mixtures (Release, ICRN)
14. ²Combustion gases

Thursday 13 September

15. Collaborative projects
 - (a) Report on existing/closing projects
 - (b) Plans for new projects
16. TPWS issues related to IAPWS monograph
17. ¹ICRN for Metastable Steam Region
18. ¹Website issues for WG's
19. Future tasks and collaborations
20. Membership
21. New Business
22. Preparation of the Formal Motion to the EC
23. Adjournment

¹ Joint session with WG IC

² Joint session with WG PCAS