THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

MEMBERS	**ASSOCIATE MEMBERS**
Australia	Argentina and Brazil
Britain and Ireland	China
Canada	Egypt
Czech Republic	France
Germany	Greece
Japan	India
New Zealand	Israel
Russia	Italy
Scandinavia (Denmark, Finland, Norway, Sweden)	Switzerland
United States of America	

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Minutes of the Virtual Meeting

of the

Executive Committee

of the

International Association for the Properties of

Water and Steam

14th and 17th September 2021

Prepared by Barry Dooley

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Minutes of the Virtual Meeting
of the
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14th and 17th September 2021

At 12:00 noon in the UK, the President of IAPWS, Professor Masaru Nakahara welcomed the Executive Committee (EC) and other IAPWS members to the Virtual Executive Committee (EC) Meeting operating on MS TEAMS. All of the Member and Associate Member countries of IAPWS were in attendance with the exception of Russia, Argentina/Brazil, Egypt, France, Greece and India. In total there were 57 people assembled for the EC meeting.

1. Adoption of Agenda

Provisional agendas had been e-mailed to all IAPWS members by the Executive Secretary from 31st July 2021. There were no additions and the final agenda forms Attachment 1 of these minutes.

2. IAPWS Business and Appointment of Committees

2.1 IAPWS Business Since Last EC Meeting, Virtual 11th September 2020

During the year since the last IAPWS EC Meeting activity took place on the following documents and with regards to IAPWS Officers:

- *Statutes and By-Laws.* 2020 IAPWS Minute 2.4 indicated that the IAPWS name and/or logo may be used in association with conferences or other events sponsored or co-sponsored by National Committees or Working Groups but only if prior approval is obtained from the IAPWS President. The IAPWS name and/or logo should not be used in a manner that gives the appearance of promoting a commercial process or entity. The document was circulated for a Postal Ballot on 21st September 2020. No objections were received by 22nd October 2020, so the new By-Law 10 became an official part of the IAPWS Statutes and By-Laws.
- *Release on IAPWS Formulation 2020 for the Viscosity of Heavy Water. 2020 IAPWS* Minute 3.1.4 indicated that the Release was finished, but feedback on the evaluation report was required. The EC authorized a Postal Ballot following final feedback and editorial committee review. The document was circulated for a Postal Ballot on 3rd December 2020. No objections were received by 3rd March 2021, so the Release became an official IAPWS document (IAPWS R17-20).
- *IAPWS Officers*. In response to 2020 IAPWS Minute 7, the US National Committee informed the Executive Secretary that Dr. Dan Friend was nominated to be the new IAPWS Vice President from 1st January 2021.

2.2 IAPWS Awards Committees for 2022

2.2.1 Honorary Fellow Award Committee

A committee of Harvey (Chairman) and Kretzschmar were selected for the 2022 Honorary Fellow award with the President and Executive Secretary as ex. Officio members.

Action: Nominations are due to the Executive Secretary by 31st January 2022.

2.2.2 Helmholtz Award Committee

The Executive Secretary reminded the EC that the Helmholtz Award selection committee for the 2022 award would consist of a member from SIAPWS (Chair) (Jensen), USA (Anderko), Australia (Henderson), BIAPWS (Caswell) and Canada (Cook).

Action: Nominations are due to the Executive Secretary by 31st January 2022.

It was noted that the 2020 (Dr. Ishiyama) and 2021 (Dr. Hellmann) Helmholtz Awardees provided Helmholtz lectures at the IAPWS Symposium following the EC Meeting. Each lecture was preceded by the IAPWS President presenting the Awards virtually and recording the citations.

2.3 Host Country for 18th ICPWS

IAPWS 2020 Virtual EC Minute 2.3 had requested the Head of the US National Committee (Friend) to report back at the 2021 EC meeting with details on hosting the 18th ICPWS. Friend indicated the following points:

- The U.S. National Committee will host the 18th ICPWS in conjunction with the 22nd Symposium on Thermophysical Properties (STP) on 23rd to 28th June 2024 at the University of Colorado Boulder campus
- Organization will involve a Local Organizing Committee (LOC) and an International Program Committee (IPC) (including IAPWS Officers and WG Chairs). Friend will act as co-chair for both conferences.
- The initial thoughts and plan for the conference are that it will follow the traditional ICPWS format modified to integrate with STP.

3. Preview by the IAPWS Week's Activities

President Nakahara reviewed the Symposium and the EC Meetings on 15th and 17th September 2021 respectively. The details are included in Attachment 2.

Following this item, the President closed the opening session of the EC at 12:35 pm in the UK.

Activities During the Week

The first day activities of the Executive Committee and the two Helmholtz Award lectures were followed by the IAPWS Symposium on Wednesday, 15th September 2021 (agenda included in Attachment 2).

Executive Committee Meeting. Friday, 17th September 2021

President Nakahara opened the continuation of the EC Meeting at 12:00 noon in the UK. All of the Member and Associate Member countries of IAPWS were in attendance with the exception of BIAPWS, Russia, Argentina/Brazil, Egypt, France and Israel. In total there were 34 people assembled for the EC meeting.

Nakahara then asked the EC if there were any additional items that should be added to the EC Agenda. None were suggested.

4. Acceptance of Minutes of Previous Meeting

President Nakahara asked for comments and changes to the minutes of the Virtual EC meeting held on 11th September 2020. No changes were noted; thus the 2020 Minutes were accepted.

5. President's Report

President Nakahara next provided his report and highlighted items of importance for the future of IAPWS and for each Working Group. The full report is Attachment 3.

6. Thermophysical Properties of Water and Steam (TPWS) Working Group (WG)

Minutes of the TPWS WG conducted before the EC meeting are in Attachment 4. TPWS Chairman Meier discussed the following items with the EC:

6.1 Release on Thermal Conductivity of Heavy Water.

The TPWS Chair informed the EC that the WG had approved the release and requested the EC to authorize a Postal Ballot following review by the Editorial Committee.

The EC approved this proposal unanimously.

6.2 Heavy Water Static Dielectric Constant

The TPWS Chair informed the EC that a suggestion had been made to develop a strategy for a new formulation for the static dielectric constant of heavy water. A Task Group had been appointed jointly with the PCAS WG consisting of Harvey and Tremaine. The Chair of PCAS, Yoshida, requested approval from the EC.

The EC approved this proposal unanimously.

6.3 ICRN-16. Thermophysical Properties of Sea Water

The TPWS Chair informed the EC that this ICRN was originally adopted in 2007, revised in 2010 and 2014, and had expired in 2019. In the absence of the Chair of the Sub-Committee on Seawater, Pawlowicz, TPWS requested the EC to extend the ICRN for another year without change of content to allow time for consideration of the next steps.

The EC approved this proposal unanimously.

6.4 ICRN-28. Thermophysical Properties of Metastable Steam and Homogeneous Nucleation.

The TPWS Chair informed the EC that this ICRN was originally adopted in 2011, renewed 2014, and had expired 2019. The ICRN is still up to date, so TPWS requested the EC to extend the ICRN for another five years (2026) with no change of content.

The EC approved this process unanimously.

6.5 ICRN-30. Thermophysical Properties of Supercooled Water.

The TPWS Chair informed the EC that this ICRN was originally adopted in 2015 and was due to expire in 2020. TPWS supports this expiry date, but this technical area is important enough that TPWS will develop a new ICRN. A Task Group had been appointed (Hellmuth (Chair), Caupin and Lago). The Task Group will prepare a closing statement for ICRN-30 and draft a new ICRN for 2022.

The EC approved this process unanimously.

6.6 TPWS Membership and Officers

The TPWS Chair proposed one new WG member:

Dr. Aleš Blahut, Institute of Thermomechanics of the CAS, Czech Republic.

The EC approved the new WG member unanimously.

The TPWS Chair also requested the EC to approve Hrubý as a second TPWS Vice-Chair effective after 2021 EC Meeting. He informed the EC that Harvey will remain as another Vice-Chair until the IAPWS 2022 Meeting.

The EC approved this new TPWS officer arrangement unanimously.

7. Industrial Requirements and Solutions (IRS) Working Group

Minutes of the IRS WG conducted before the EC meeting are in Attachment 5. The IRS Chairman Okita indicated that there were no items that needed EC approval.

8. Sub-Committee on Seawater (SCSW)

Unfortunately, the SCSW Chair, Pawlowicz, could not be present for the EC meeting.

9. Physical Chemistry of Aqueous Systems Working Group (PCAS)

Minutes of the PCAS WG conducted before the EC meeting are in Attachment 6.

IRS Chairman Yoshida discussed the following items with the EC:

9.1 Heavy Water Static Dielectric Constant

The PCAS Chair indicated that the joint task group with TPWS had already been approved by the EC (Minute 6.2).

9.2 PCAS Membership

The PCAS Chair proposed four new WG members:

Dr. Tatsuya Ishiyama, University of Toyama, Japan
Dr. Jacy Conrad, Idaho National Laboratory, USA
Miss Lucy Platt, National Nuclear Laboratory, UK
Dr. Chris Alcorn, Los Alamos National Laboratory, USA

The PCAS Chair also informed the EC that Dr. Andrey Plyasunov, Russian Academy of Sciences, Russia had requested to be removed from the WG.

The EC approved these new WG member changes unanimously.

9.3 On-going and Future Task Groups

The PCAS Chair informed the EC of the following activities:

a) Guideline on self-diffusion coefficient. Led by Yoshida, in collaboration with TPWS. In progress.
b) Guideline on ionization constant of light water. Proposed in PCAS separate meeting by Tremaine and Arcis as a possible future Task Group. There is a plan to set up a task group in 2023.
c) Geothermal White Paper. Joint Japan and New Zealand meeting with PCAS/PCC/IRS WG members had been held in April 2021.
d) Acid dew point. Led by Okita, in collaboration with IRS. There is a plan to propose an ICRN.

9.4 Possible New Sub-committee or Working Group

The PCAS Chair wanted to inform the EC that a discussion had taken place on the possibility of expanding IAPWS activities into the area of radiation chemistry, especially at high temperatures (experimental and modeling). PCAS will report to the EC at the 2022 meeting.

10. Power Cycle Chemistry Working Group (PCC)

Minutes of the PCC WG conducted before the EC meeting are in Attachment 7.

PCC Chairman Rziha discussed the following items with the EC:

10.1 Technical Guidance Documents (TGD)

The PCC Chair provided the EC with the following updates on the TGD that were either in preparation or being considered at the 2020 EC meeting:

a) Chemistry in Geothermal plants. Development of White Paper (pre-TGD) remains active.
b) Corrosion Product Sampling, Monitoring for Flexible and Fast Starting Plants. Development of White Paper remains active, but the pandemic has restricted any plant monitoring.
c) Water Treatment of Flue Gas Condensate. Development of White Paper remains active.
d) Chemistry for Electrode Boilers. This new TGD will initially prepare a White Paper through a joint Task Group between SIAPWS and New Zealand.
e) FFS application in Nuclear Plants. There had been no activity on this White paper since the Banff meeting, but new writing assignments have now been put in place.
f) Demin Water Integrity. There has been no significant activity on this TGD over the last five years so PCC decided to retire the development.
g) Condensate Polishing Plants for Combined Cycle / HRSG plants. There has been no activity for a number of years, but PCC agreed to keep this activity open until the 2022 meeting. If there is still no activity, it will be retired.

h) Informed or Smart Alarms. PCC decided to retire this activity as an adjunct to the IAPWS TGD on Instrumentation, but it was agreed that this important TGD will be reviewed and updated as appropriate.

10.2 International Collaborations

The PCC Chair informed the EC that there were no new Collaborations proposed and indicated that the Boiler / Corrosion collaboration between Canada and New Zealand was continuing but had been delayed due to the pandemic.

10.3 PCC Membership and Officers

The PCC Chair proposed three new WG members:

Dr. Hugues Arcis, National Nuclear Laboratory Limited UK
Mrs. Lucy Platts, National Nuclear Laboratory Limited UK
Mrs. Maria del Mar Nogales Lopez, SWAN AG, Switzerland.

The EC approved these new WG member changes unanimously.

The PCC Chair next indicated that he would be stepping down as Chair after 10 years. He proposed Vice Chair Addison to become the new PCC Chairman following the EC Meetings. The PCC had suggested that he stays on as Vice Chair for a year for continuity and support. Vice Chair McCann will remain in this position,

The EC approved these new PCC officer arrangements unanimously.

IAPWS Vice President Friend, on behalf of IAPWS and the EC, thanked Rziha for his excellent service as PCC Chair.

11. Editorial Committee Report

Editorial Committee Chairman Harvey reported that in the preceding year, the Editorial Committee (Harvey, Cook and Cooper) had reviewed the *Release on Viscosity of Heavy Water* mentioned in Minute 2.1, and were currently reviewing *Release on Thermal Conductivity of Heavy Water* mentioned in Minute 6.1.

12. Membership and Associates

12.1 Report on Membership

The Executive Secretary reported that only BIAPWS had not paid the 2021 dues by the end of August.

12.2 Reports on Current Associate Members

Status Report on IAPWS Associate Member, Egypt. The Head of the Egypt National Committee, Khalifa, unfortunately was not present at the EC but had indicated to the Executive Secretary that he would provide a status report following the meeting.
Status Report on IAPWS Associate Member, Greece. Mr. Antony Thanos indicated that he was the new Chair of HIAPWS and that the National Committee would be organizing a symposium later in 2021.

Status Report on IAPWS Associate Member, India. The Executive Secretary reported that the Head of the India National Committee (INDIAPWS), Bhattacharyya, had sadly passed away. The India National Committee has been reorganizing and will report to the Executive Secretary.

Status Report on IAPWS Associate Member, Italy. The head of the Italian National Committee, Lago, reported that the Italian National Committee is planning to become a full member of IAPWS and has contacted interested industries and universities.

Status Report on IAPWS Associate Member, Switzerland. A report of the Switzerland National Committee (SCPWS) is provided as Attachment 12. Swiss Delegate Werder indicated that no team of sponsors had been assembled to commit on a mid- or longterm basis to a regular Swiss membership fee. Activities were therefore limited to a few individuals. Due to COVID-19, no activities as planned had taken place. The board of SCPWS is currently planning for 2022 to find new participating institutions in Switzerland. Marco Lendi resigned from the Presidency at the end of 2020. The Swiss National Committee will provide information to the Executive Secretary on the new head of the SCPWS by the end of 2021. It is therefore requested to extend the Associate Membership for another term.

Status Report on IAPWS Associate Member, Israel. (Report provided to the Executive Secretary after the close of the EC Meeting by the Head of ISRAPWS, Nussbaum). In the last 10 years the Israeli electrical system has changed dramatically. There are more power plants working on Israeli gas from the sea and less power plants working on coal. In 2020, 24% of the power came from coal fired plants but by 2025 there will only be 2%. There will be an increase in private power plants from 42% today to around 69% in 2025. There are new small combined cycles built inland. ISRAPWS is trying to find a way around all of these changes. They plan the next symposium in November 2021 with more than 30 participants, most from the power plants but will also include chemists, engineers, and operators as well as regulation and academic people. Nussbaum is trying to attract people from related disciplines such as water treatment, seawater desalination, regulation, laboratories and universities. ISRAPWS is also addressing the financial side of the National Committee.

13 Executive Secretary's Report

13.1 IAPWS Bank Accounts, Financial, Auditors and IAPWS Dues

The Executive Secretary reported that IAPWS is on a sound financial footing with currently about £100,000.00GBP in total in the UK and US bank accounts. The status as at 4th September 2021 in the bank accounts had been provided to the Head of each IAPWS Member country prior to the EC meeting.

The Executive Secretary next reported that the 2020 financial statements had been forwarded to the IAPWS Auditors in January 2021. Professor Savarik in Czech Republic and Dr. Delfs of VDI in Germany had reviewed and approved the financial statements. These approvals had also been provided to the Heads of each IAPWS Member National Committee prior to the EC meeting.

The Executive Secretary proposed that these organizations be re-appointed to act as auditors The Head of the Czech Republic National Committee, Nemec, responded positively. The German Delegate, Kretzschmar, indicated that he will respond by the end of November 2021.

The EC Approved these Actions Unanimously.

The Executive Secretary proposed to the EC that the dues structure for member countries remains unchanged for 2022.

The EC Unanimously Agreed to this Proposal.

13.2 Time and Place of the 2022 and 2023 IAPWS Meetings

2022 IAPWS Meetings. The Head of the New Zealand National Committee, Addison, indicated that NZAPWS are ready and waiting to hold the 2022 IAPWS meetings in New Zealand but the restrictions imposed by the Government might preclude this. So, at this time he couldn't definitively indicate that the 2022 IAPWS Meetings could be held in New Zealand. This generated some discussion from the EC in terms of alternate arrangements and dates. Possibilities discussed were: combined virtual and live meetings; separate meetings (live or virtual) of separate WGs; and moving the dates for a live meeting towards the end of 2022. The consensus of the EC was to wait until later in 2021 to decide how IAPWS should plan for 2022.

2023 IAPWS Meetings. The Head of the Italian National Committee (NC), Lago, indicated that the Italian NC confirms that at the present time the 2023 meetings are planned to be held in Turin. Full details will be provided at the 2022 EC.

14. IAPWS Awards

14.1 Helmholtz Award.

The IAPWS President indicated that the 2020 Award had been given to Dr. Tatsuya of the University of Toyama, Japan, and that the 2021 Award had been given to Dr. Robert Hellmann, Helmut-Schmidt University, Germany.

The Helmholtz Award Committee for 2022 had been formulated in Minute 2.2.1.

14.2 Honorary Fellow Award.

The IAPWS President also indicated that there had been two Awardees for 2021: Dr. Jan Hruby of the Czech Republic and Dr. Karsten Thomsen of SIAPWS.

15. Other Business

15.1 Storage of Documents from ICPWS

The Executive Secretary added this item to the EC Agenda during the week as it had been reported that the Website for the 17th ICPWS had disappeared along with the content. A number of the EC present provided some discussion on possible solutions. It was finally suggested that the USA in preparing for and running the 18th ICPWS provide an indication of how materials from the conferences could become a permanent record for IAPWS.

15.2 Reports from National Committees.

Written reports on progress in member countries provided after the EC meeting are attached to these minutes as follows:

Canada	Attachment 8
Czech Republic	Attachment 9
Germany	Attachment 10

Japan	Attachment 11
Switzerland	Attachment 12
USA	Attachment 13

15.3 List of Members

An up-dated list of members of the Executive Committee, Working Groups, and Honorary Fellows will be developed by the Executive Secretary following the Virtual EC Meeting. This will be forwarded electronically to the Head of each National Committee and the Working Group Chairs.

16. Closing Remarks and Adjournment

No further business was raised by the EC. The President thanked everybody for participating at this EC meeting. The 2021 EC meeting was closed at 1:56 pm in the UK.

AGENDA for the EXECUTIVE COMMITTEE (EC) of IAPWS

Tuesday, 14th September 2021. Opening Plenary Session (12:00 – 12:30 UK Time)

Opening Remarks, Welcome and Introductions by IAPWS President M. Nakahara

1. Adoption of Agenda
2. IAPWS Business and Appointment of Committees
   - 2.1 IAPWS Business since Last EC Virtual Meeting, September 2020
   - 2.2 Evaluation Committee on International Collaboration
   - 2.3 IAPWS Awards Committees for 2022 (Honorary Fellow, Helmholtz)
   - 2.4 Report by USA Chairman Friend on 18th ICPWS
   - 2.5 Any other business requiring discussion
3. Preview of Week's Activities by IAPWS President

Friday, 17th September 2021. Executive Committee Meeting. (12:00 – 2:00 UK Time)

4. Acceptance of Minutes of Previous Meeting
5. President's Report
6. Report and Recommendations of TPWS Needing EC Approval
7. Report and Recommendations of IRS Needing EC Approval
8. Report and Recommendations of SCSW Needing EC Approval
9. Report and Recommendations of PCAS Needing EC Approval
10. Report and Recommendations of PCC Needing EC Approval
11. Editorial Committee Report
12. Membership and Associates
    - 12.1 Report on Membership
      Including Members Defaulting on Dues.
    - 12.2 Reports of Current Associate Members
13. Executive Secretary's Report
    - 13.1 IAPWS Bank Accounts, Financials, Auditors and Dues
    - 13.2 Time and Place of 2022 (New Zealand) and
      2023 (Italy) Meetings.
14. Guidelines, Releases, Certified Research Needs, and International Collaborations
    - 14.1 International Collaborations
15. IAPWS Awards
    - 15.1 Helmholtz Award Committee
    - 15.2 Honorary Fellowship
16. New Business. Other items raised during the IAPWS week
    - 16.1 Storage of Documents from ICPWS
17. Adjournment

IAPWS

Barry Dooley
17th September 2021

IAPWS Virtual Executive Meetings and Symposium

14th – 17th September 2021

All Times are UK Times

Tuesday, 14th September 2021.

12:00 **Opening *EC Meeting.***
EC Agenda Published Separately
Chair: IAPWS President Masaru Nakahara, Kyoto University, Japan

Helmholtz Awards Symposium

Chair: IAPWS President Masaru Nakahara, Kyoto University, Japan

12:45 ***Helmholtz 2020 Award Lecture***
Molecular Dynamics Study of Transport, Structure and Spectroscopy at Liquid Interfaces
Tatsuya Ishiyama, University of Toyama, Japan.

13:30 ***Helmholtz 2021 Award Lecture***
Thermophysical Properties of Water Vapor and its Mixtures with Other Gases from First-Principles Calculations
Robert Hellmann, Helmut-Schmidt University, Hamburg, Germany.

Wednesday, 15th September 2021.

IAPWS Virtual Symposium

12:00 **Thermophysical Properties of Water and Steam (TPWS)**
The IAPWS-95 Reference Equation of State for Water and its Future Replacement
Allan Harvey, NIST, USA.

12:30 **Industrial Requirements and Solutions (IRS)**
Advances in Large Eddy Simulation of Non-equilibrium Condensation in Steam Turbines
Francesca di Mare, Ruhr-Universität, Bochum, Germany

13:00 **Physical Chemistry of Aqueous Solutions (PCAS)**
Water-Polymer Interactions Analyzed by All-Atom MD Simulations: Fugaku Supercomputer Project toward Materials Design
Nobuyuki Matubayasi, Osaka University, Japan

13:30 **Power Cycle Chemistry (PCC)**
Film Forming Substances (FFS): The Path towards an ICRN
Barry Dooley, Structural Integrity, UK and
David Addison, Thermal Chemistry, New Zealand.

14:00 **Open Discussion**

Friday, 17th September 2021.

12:00 **IAPWS *EC Meeting.***
Chair: IAPWS President Masaru Nakahara, Kyoto University, Japan

IAPWS President, Masaru Nakahara Report to IAPWS EC
17th September 2021

Dear Colleagues:

Ladies and gentlemen. Welcome to you all. The delegates from the full member countries and from the associated member countries, and from other non-member countries. I am happy to have a chance of expressing my thoughts about the present and future states of IAPWS, The International Association for the Properties of Water and Steam. The key word WS used here means water and steam which are of substantial importance for our living, in particular, through (electricity) power generation.

I express my sincere thanks to the chairs of the IAPWS Working Groups; TPWS, (Thermophysical Properties of Water and Steam), IRS (Industrial Requirements), SCSW (Sub-committee on Seawater), PCAS (Physical Chemistry of Aqueous Systems), and PCC (Power Cycle Chemistry). All the chairs have worked elaborately to make creative contributions to IAPWS. Thank all the participants here. You have joined us to stimulate and deepen our discussions in the IAPWS September 2021 meetings. The virtual IAPWS meetings of this year have been made so successful by your great contributions. I hope you have learned a lot about our products useful for you. Consider how best to utilize such IAPWS products as Releases, Guidelines, and Technical Guidance Documents, and IAPWS Certified Research Needs (ICRN). All of these are characteristic of the IAPWS business. The useful IAPWS products are now popular all over the world. You can make access to the IAPWS website when you have any interest or question about WS. I am sure you can learn about the treatment, handling, and monitoring of WS as well as the scientific formulation and meaning. IAPWS has so many good engineers and scientists. Do not hesitate to try communicating with them.

Hot WS including supercritical water at high temperature is the most important working substance for generating (electric) power. The thermal WS energy is transformed through boilers and turbines. Hot WS are interacting with metals at the interface or on the surface over a wide range of temperature. Now where are we going in the WS business? Is it the same as the past? Our old primitive lifestyle heavily depended on human working with hands and feet. Now most of them have been replaced by the motors working and driven through electricity or electrons. Progress in the modernization of our society has been assisted by IAPWS, and we hope this continues in future. In many industrialized countries the government has announced that our cars are to be of the EV type, electric vehicle that are driven by electricity. As you know the human beings are desirous and the population on Earth dramatically increases. On the other hand, people want no carbon emission or carbon neutral society, probably in relation to the climate changes, although all planets are cooling on the long-time scale. Luckily, Earth is rich in WS, but other planets like Mercury and Venus have the air or cloud dominated by CO_2.

Human beings are greedy and always want something more and better despite the explosive increase of the population on Earth. We don't like the ancient lifestyle in any sense What should we do? How can we survive? All of us are responsible for this serious polarization, more energy and less carbon emission.

Here I want to say something from the viewpoint of IAPWS. All energies, thermal or nuclear, come from the Sun. Sun continues to provide carbohydrates $[C_6 \cdot (H_2O)_6]_n$ containing carbon and hydrogen atoms through the conversion of CO_2 and H_2O, the former as the carbon C source and the latter as hydrogen H source. They were buried for billion years and transformed into fossils through dehydration, such as coals, oils, and gases. We have used them in a short time as fuel since the Industrial Revolution that occurred four hundred year ago. Now we need to have some more revolution. Fuels are changing from coal mainly composed of carbon atoms to fuels with less carbons like methane and ultimate fuel

hydrogen. Here I'll mention two things for the IAPWS future.

One is "interfacial phenomenon engineering" and the other is "computational skills". Historically, IAPWS has been moving on from pure WS to seawater. From single component to multi-component aqueous systems. We have paid attention mainly to soft materials. Now it is time for us to pay more attention to hard materials in the solid state and the interfaces between the soft and hard materials. In the power cycle of boiler and turbine WS are in contact with metals. There occurs corrosion under the severe conditions during the long-time operation. Recently IAPWS has stressed the importance of the study on the film-forming substances FFS like alkylamines. Film can increase lifetime of metals used for the boiler tubes and turbine blades.

Combining renewable energy with the traditional one is an urgent issue to protect the global environments. This affects the cost and safety of the power supply system. It is essential to improve the efficiency as much as possible in the switching from the traditional fossil power to another. The key is the security of the safety and stability. Frequent shutting down and starting up of a fossil plant for tuning the supply are unavoidable operations. Then the maintenance becomes challenging because undesirable gaseous corrosives such as oxygen and carbon dioxide can be brought into the WS cycle induced by temperature and pressure changes. Developing effective corrosion inhibitors is an urgent demand. In recent years, application of film forming substances (FFS) have been proposed and more fundamental studies are wanted as emphasized by IAPWS; that is the Technical Guidance Document (TGD) on the application of FFS in WS power plants and industrial steam generators. By introducing FFS, a hydrophobic film is thought to be formed on the inner surface of tubes in the WS cycle. Interface science and technology are to be considered in order to get insight into what and why it happens. We are interested in the chemical reaction dynamics, reaction pathways, reaction mechanism, liquid and solid nucleation processes, and chemical structure of films formed at the interface.

Next we can focus on the expansion of the "computational approach". This machine-learning is taking place instead of the analytical solution one and has been widely used in many complicated fields. Analytical solutions are usually based on assumptions and approximations. Practical problems often have no analytical solutions. We need to rely upon simple and deep approach with much less assumption restrictions. In this case, the computational approach can be more powerful with the aid of the rapid advancement of computer machines. Large-scale Molecular Dynamics simulation is hoped to make it possible to see what is going on in the power plant in a predictive way and from the microscopic viewpoint. In addition, the frequent and quick shut-down and start-up mentioned above can be controlled safely by AI. I believe you have enjoyed some of these stories in these IAPWS meetings.

IAPWS Thermophysical Properties of Water and Steam WG
Virtual meeting, 31 August and 1 September 2021

NOTE: 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 at 15:00 Central European Summer Time on Tuesday, August 31, 2021 by the TPWS Chair, Karsten Meier. The draft Agenda was approved. Allan Harvey was appointed Clerk of Minutes for TPWS.

3. Potential International Collaborative Projects

No new Collaborative Project was suggested at TPWS.

4. Presentation from B. Semrau and R. Span: "Consistent combination of accurate property models for CCS-applications including brines and Helmholtz energy mixture models – from seawater to more concentrated brines." The work, still in progress, involves combining a Helmholtz mixture equation-of-state model (for example, for H_2O-CO_2) with a Gibbs energy model for a brine, such as the TEOS-10 seawater model or the Pitzer electrolyte model.

5. Presentation from J. Stefanski, B. Issenmann, and F. Caupin: "Shear and bulk viscosity of water up to 1.3 GPa." The work used dynamic differential microscopy, with polystyrene spheres as Brownian particles, to obtain the shear viscosity, and then Brillouin spectra were used to obtain the bulk viscosity. Future plans include measuring at higher temperatures, measuring heavy water, and measuring aqueous salt solutions.

6. Presentation by F. Fehres and S. Rudtsch, "Measurements of the speed of sound in sea water." The data extend to 80 °C and somewhat high pressures at a variety of salinities, with relatively low uncertainties, and fill what had been a significant gap in the literature database. A publication is in preparation.

7. Report of Task Group on Surface Tension of Ordinary Water. This was presented by K. Meier on behalf of J. Kalova. New data have been published by Kalova and Mareš on the surface tension of supercooled water. At the lowest temperatures (near –32 °C), the extrapolated IAPWS correlation seems systematically low. In the discussion, it was noted that some comparisons with measurements from the group in Prague need to be made, and that for practical purposes the greatest need is for accurate experimental data above 350 K as stated in ICRN-31.

8. Status Report of the Working Group on the Relative Humidity of the Joint Committee on Sea Water (O. Hellmuth, R. Feistel). A number of recent papers were described, including a review on the role of water in the energy balance of the climate system and multiple papers related to the concept of relative fugacity.

9. Heavy Water Properties

9.1 Presentation by G. Beltramino, R. Cuccaro, L. Rosso, and V. Fernicola: "Measurements of the vapor-liquid equilibrium along the saturation line of supercooled heavy water

between 256 K and 286 K." The data have been published, and are in good agreement with values from the (extrapolated) IAPWS equation of state for heavy water.

9.2 Presentation by J. Cox, J. Young, A. Harvey, and P. Tremaine: "Progress on a Formulation for the Static Dielectric Constant of Heavy Water." A strategy for correlating this property, with some guidance from the existing IAPWS formulation for the dielectric constant of ordinary water, was outlined.

9.3 **The WG appointed (jointly with PCAS) a Task Group on the Static Dielectric Constant of Heavy Water, consisting of Allan Harvey and Peter Tremaine.** The Chairs of the WGs are authorized to appoint an Evaluation Task Group during the year if work on the new formulation proceeds to the point where evaluation is needed.

9.4 Report of Task Group for Heavy Water Transport Properties on the Formulation for the Thermal Conductivity of Heavy Water (J. Sengers, M. Assael, M. Huber, R. Perkins). The new formulation and its performance were summarized.

9.5 Report of the Evaluation Task Group for the Release on the Formulation for the Thermal Conductivity of Heavy Water (K. Meier). The Evaluation was summarized, and the Evaluation Task Group recommended adoption of the Release.

9.6 **The WG unanimously recommended adoption of the Release. The IAPWS Executive Committee is requested to authorize a Postal Ballot for the Release after it is reviewed by the Editorial Committee.**

10. IAPWS Certified Research Needs (ICRNs)

10.1 ICRN 16: Thermophysical Properties of Seawater (R. Pawlowicz). In the absence of R. Pawlowicz, **the WG requests that the ICRN be extended until 2022 to allow time for consideration of the next steps**.

10.2 ICRN 28: Thermophysical Properties of Metastable Steam and Homogeneous Nucleation (J. Hrubý). **The WG requests that this ICRN be extended for an additional 5 years, with no change in the content.**

10.3 ICRN 30: Thermophysical Properties of Supercooled Water (O. Hellmuth). There has been much recent work in this field. It was decided to allow the current ICRN to expire, but that the area was important enough that a new ICRN should be produced. **A Task Group on Thermophysical Properties of Supercooled Water was appointed consisting of O. Hellmuth (Chair), F. Caupin, and S. Lago. The TG should prepare a Closing Statement for ICRN 30, and draft a new ICRN on this topic for consideration at the 2022 IAPWS meeting.**

11. Other Business

11.1 Report on International Collaborative Projects. Nothing to report on this item.

11.2 Development of an IAPWS Recommendation for the Vapor Pressure of Supercooled Water Based on the Existing Guideline on Thermodynamic Properties of Supercooled Water. A. Harvey described a plan to produce a simple correlation for the vapor pressure of supercooled liquid water based on the thermodynamic formulation in the existing IAPWS G12-15: Guideline on Thermodynamic Properties of Supercooled Water. A Task Group on this topic was already appointed in 2017, consisting of A. Harvey, V. Holten, and R. Feistel. The Chair of the WG was authorized to appoint an Evaluation Task Group during the year if work on the new formulation proceeds to the point where evaluation is needed.

12. Membership

Aleš Blahut (Czech Republic) was unanimously elected as a new TPWS member.

13. Election of Vice-Chair

J. Hrubý was elected as a Vice-Chair, effective upon approval by the EC. K. Meier remains as Chair, and A. Harvey remains as an additional Vice-Chair for the next year.

14. Contribution to Press Release

The Chair was assigned to prepare the contribution to the Press Release.

15. 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.

16. Adjournment

The meeting was adjourned at approximately 17:40 Central European Summer Time on Wednesday, September 1.

TPWS Attachment A
Agenda for the IAPWS Working Group
Thermophysical Properties of Water and Steam (TPWS)
Virtual Meeting, August 31-September 1, 2021

Tuesday, August 31, 2021

1. Opening Remarks; Adoption of Agenda
2. Appointment of Clerk of Minutes
3. Potential International Collaborative Projects
4. B. Semrau and R. Span: Consistent combination of accurate property models for CCS-applications including brines and Helmholtz energy mixture models – from seawater to more concentrated brines
5. J. Stefanski, B. Issenmann, and F. Caupin: Shear and bulk viscosity of water up to 1.3 GPa
6. F. Fehres, S. Rudtsch: Measurements of the speed of sound in sea water
7. Report of the Task Group for the Surface Tension of Ordinary Water (K. Meier on behalf of J. Kalová)
8. Status Report of the Working Group on the Relative Humidity of the Joint Committee on Sea Water (O. Hellmuth, R. Feistel)

Wednesday, September 1, 2021

9. Heavy Water Properties:
   - 9.1 G. Beltramino, R. Cuccaro, L. Rosso, and V. Fernicola: Measurements of the vapor-liquid equilibrium along the saturation line of supercooled heavy water between 256 K and 286 K
   - 9.2 J. Cox, J. Young, A. Harvey, and P. Tremaine: Progress on a Formulation for the Static Dielectric Constant of Heavy Water
   - 9.3 Appointment of a Task Group “Static Dielectric Constant of Heavy Water”
   - 9.4 Report of Task Group for Heavy Water Transport Properties on the Formulation for the Thermal Conductivity of Heavy Water (J. Sengers, M. Assael, M. Huber, R. Perkins)
   - 9.5 Report of the Evaluation Task Group for the Release on the Formulation for the Thermal Conductivity of Heavy Water (K. Meier)

9.6 Formal consideration of the Release on the Thermal Conductivity of Heavy Water

10. IAPWS Certified Research Needs (ICRNs)

10.1 ICRN 16: Thermophysical Properties of Seawater (R. Pawlowicz)

10.2 ICRN 28: Thermophysical Properties of Metastable Steam and Homogeneous Nucleation (J. Hrubý)

10.3 ICRN 30: Thermophysical Properties of Supercooled Water (O. Hellmuth)

11. Other Business

11.1 Report on International Collaborative Projects

11.2 Development of an IAPWS Recommendation for the Vapor Pressure of Supercooled Water Based on the Existing Guideline on Thermodynamic Properties of Supercooled Water (A. Harvey, V. Holten, R. Feistel)

12. Membership

13. Election of Vice-Chair

14. Contribution to Press Release

15. Preparation of the Formal Motion to the EC

16. Adjournment

August 31, 2021

Karsten Meier (Chair), A.H. Harvey (Vice-Chair)

Attachment 5

Minutes of the IAPWS working group IRS, On-line second meeting, 23 August 2021

(Numbering of the topics follows IRS agenda)

1. The Chair, Nobuo Okita, opened the on-line (Cisco Webex) IRS joint meeting at 10:05 am (CEST) on 23 August 2021.

2. Appointed Shigeki Senoo as a clerk of minutes.

3. New item for considering IRS task group (Francesca di Mare)

Prof. Dr. Francesca di Mare propose and explain the energy storage system, including innovative energy supply cycle and turbomachinery. The purposes of the TG are discussion and clarification of system with potential issues to install energy storage system. Other members agree the necessity of innovative energy storage system under increasing renewable energy environment.

TO DO:

Prof. Dr. Francesca di Mare send the presentation material to participants.

WG continuously discuss to launch the TG.

4. Status of each task of Industrial Requirements and Solutions

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

N. Okita explain the status.

TO DO:

After discussion with PCAS on 26th August and so on, the list of category is to be updated.

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

N. Okita reported no progress and there were no other suggestions by other members.

TO DO:

Continue keeping the TG active.

4.3 Report of the joint Task Group "Wet Steam Data from Operating Turbines" (*S. Senoo*, N. Okita, A. Anderko) [Joint with PCAS]

S. Senoo reported no progress.

S. Senoo presented a paper which Mitsubishi Power and Mitsubishi Heavy Industries made a presentation of "Investigation of moisture removal on last stage stationary blade in actual steam turbine" in ASME turbo expo 2021. The paper have relevance to the task group and explained a newly developed water film removal structures to reduce erosion damage in the last stage

blades of steam turbines. The effectiveness of the developed slit was verified by measurement in an operating 105MW steam turbine of gas turbine combined cycle power plant.

TO DO:

Action plan to ask other WG members to cooperate.

4.4 Report of the joint Task Group on ICRN for acid gas dew points (*N. Okita*, S. Senoo, T. Němec) [Joint with PCAS]

N. Okita summarized the current status and presented new progress by using a presentation material for the virtual event of ASPEN to be held in September. Updated information includes the survey result of the dew point calculation by ASPEN model at 0.01 ppm SO3 and Model 3 is the most preferable same as the previous result. Need more investigation below 0.01 ppm and other methods of simulation.

N. Okita suggested next steps, mentioning tracing data, survey of data below 0.01 ppm and possible simulation method discussed with PCAS. Prof. Dr. Span seconded discussion with PCAS.

TO DO:

N. Okita send the presentation material to participants.

Review and discuss the Aspen model and other methods, then decide to continue simulations. Consider cooperation with PCAS on drafting ICRN. Trace data of the dew point. Cooperate on TGD with PCC.

4.5 Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, Francesca di Mare, *D. Addison*, S. Terada) [Joint with PCC]

N. Okita reported no progress and there were no other suggestions by other members.

TO DO:

Keep up with D. Addison to progress.

5. IRS Other Business: No other business.

6. IRS Membership: No change

7. IRS Formal motion to the EC will be prepared by the WG chair: No item for the formal motion

8. IRS meeting was adjourned 23 August 2021, about 11:30.

Attachment 5

Agenda for the IAPWS Working Group
Industrial Requirements and Solutions (IRS)
On-line Meeting, August 23, 2021

1. Opening Remarks; Adoption of Agenda
2. Appointment of Clerk of Minutes
3. New item for considering IRS task group (Francesca di Mare)
4. Status of each task of industrial Requirements and Solutions
   - 4.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, chairs or representatives of other WG)
   - 4.2 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)
   - 4.3 Report of the joint Task Group "Wet Steam Data from Operating Turbines" (S. Senoo, N. Okita, A. Anderko) [Joint with PCAS]
   - 4.4 Report of the joint Task Group on ICRN for acid gas dew points (N. Okita, S. Senoo, T. Němec) [Joint with PCAS]
   - 4.5 Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, Francesca di Mare, D. Addison, S. Terada) [Joint with PCC]
5. Other Business
6. Membership
7. Preparation of the Formal Motion to the EC
8. Adjournment

July 20th, 2021
N. Okita (Chair)

PCAS WG Minutes

On-Line (MS Teams), August 27, 2021, 12:00 – 14:00 (British Summer Time)

K. Yoshida – chairman, H. Arcis – vice-chair

1. Adoption of agenda

Draft agenda has been sent to PCAS members by PCAS chair K. Yoshida on August 4, 2021. No objections have been raised by PCAS members. The revised draft agenda was presented by K. Yoshida on the day of the meeting with minor updates such as information about the attendees. No objections have been raised by the attendees. Agenda has been approved.

2. Appointment of clerk of minutes

T. Němec was appointed clerk of the minutes.

3. Approval of minutes from 2020 meetings

The minutes of 2020 PCAS meetings (available online http://www.iapws.org/minutes/2020/Minutes2020.pdf) have been approved.

4. Report on 2021 PCAS Symposium

K. Yoshida reported on the number of participants of the 2021 PCAS Symposium held online on August 26, 2021. Total number of participants was 32, from Japan (13), USA (4), Czechia (3), UK (3), Canada (2), Germany (2), Russia (2), Australia, Sweden. Most participants from Japan were from industry, interested in power plant chemistry. Prof. M. Nakahara has characterized the symposium as a very successful event. Members from other working groups attended as well. The symposium idea was suggested originally by H. Arcis to promote PCAS activities and attract new researchers. K. Yoshida will report on the symposium to Executive Committee.

5. Self-introduction and reports on PCAS-related activities

Attendees have introduced themselves and their research interests:

(1) Canada:

Prof. Peter Tremaine (University of Guelph): high temperature water chemistry, thermodynamic/spectroscopic measurements of high temperature aqueous solutions, applications to CANDU primary cooling chemistry, small modular reactor water chemistry, nuclear waste management, deep underground spent fuel repository

Dr. Jane Fergusson (University of New Brunswick): molten salt chemistry, no PCAS related activities to report.

(2) Japan:

Prof. Masaru Nakahara (Kyoto University): kinectic studies of film forming amines
Prof. Nobuyuki Matubayasi (Osaka University): theory and computation of aqueous systems, Japan supercomputing project, water/polymer systems relevant to desalination
Dr. Ken Yoshida (Tokushima University): reaction and adsorption of film forming amines, NMR analysis, infrared/XPS analysis of surface amines

(3) Czech Republic:

Dr. Tomáš Němec (Institute of Thermomechanics): theoretical studies and molecular dynamic simulations of nucleation processes in water vapor, hydrogen technologies with focus on hydrogen fuel cells and electrocatalytic nanomaterials for fuel cell electrodes
Dr. Milan Sedlář (Sigma Research and Development Institute): cavitation and multi-phase flow, cavitation at high temperatures, thermal effects of cavitation
Dr. Meenakshi Seshadhri Garapati (Institute of Thermomechanics): water management in hydrogen fuel cells, experimental evaluation of electrocatalytic activity of nanomaterials

(4) United Kingdom:

Dr. Hugues Arcis (National Nuclear Laboratory): supporting commercial activities on PWR, BWR reactors, working on SMR design developed in UK
Ms. Lucy Platts (National Nuclear Laboratory): water radiolysis modelling, modelling and experimental work to support European DEMO fusion concept and SMR design developed in UK

6. Possibility of ICRNs

K. Yoshida gave details about the concept of IAPWS' ICRNs (http://www.iapws.org/icrn.html).

No new ICRNs have been proposed for 2021.

N. Okita (IRS WG) is planning to issue an ICRN about sulfuric acid dew point jointly with PCAS WG. A draft of the ICRN is not ready yet.

P. Tremaine stressed the need to develop a new formulation for the sodium chloride EOS, similar to that of Don Archer, to support experimental work such as solution density measurements. Archer's equation is based on Hills' EOS for water and older formulation for the water dielectric constant and it would be useful to have a new EOS compatible with the modern formulations recommended by IAPWS. This activity will be discussed with A. Harvey (TPWS WG) to issue an ICRN possibly in 2022.

7. International collaboration

No international collaboration activities have been proposed. Deadline for 2021 application to Executive Committee is September 6. K. Yoshida mentioned that if any member would like to apply for the next year or later, it would be better to let the Chair know as soon as possible and allow enough time to elaborate on the application.

8. Discussion of future activities of PCAS

One of the 2021 PCAS symposium objectives was to attract new PCAS members and new research topics.

H. Arcis asked whether IAPWS had historically supported radiation chemistry and whether it would be possible and of interest to expand IAPWS activities to the area of radiation chemistry, especially at high temperatures (experimental and modelling). P. Tremaine explained this has not been part of IAPWS original mandate for historical reasons. H. Arcis asked whether there might be a case to be made to create a new subcommittee or working group. P. Tremaine suggested a couple of contacts: Greg Horne at INL, Craig Stuart at CNL and Khash Ghandi at U of Guelph. New contacts are welcome to form a broader international collaboration team. Hugues Arcis explained NNL would be interested in such collaboration. K. Yoshida mentioned interest into the solubility of ammonia in water, which was discussed during the 2021 Japan national committee meeting.

(Addendum) After the meeting, K. Yoshida and H. Arcis emailed B. Dooley and M. Nakahara to ask their opinion of the possibility of creating a new Subcommittee of radiation chemistry. B. Dooley mentioned the history of the setup of SCSW and stated that the key is to attract and gather scientists involved in the radiation chemistry. B. Dooley stated that, once PCAS can gather them, the questions can be raised as to whether IAPWS is interested in this area of work and whether there is interest in forming an IAPWS sub-committee of PCAS or a separate group.

9. Discussion of the possibility of releases and guidelines

(1) A joint PCAS/TPWS Task Group to work on developing a formulation for the static dielectric constant of heavy water proposed by Dr. Allan Harvey (NIST, USA) and Prof. Peter Tremaine (University of Guelph, Canada). P. Tremaine explained the need for dielectric constant formulation above 100 °C for the purpose of CANDU primary cooling loop chemistry modeling. Data have been collected from groups working in the field by A. Harvey. Functional form of the new formulation was presented, a deviation function from light-water formulation is a possible approach. Task group proposal will be submitted to Executive Committee by K. Yoshida.

(2) A joint PCAS/TPWS Task Group to work on developing a formulation for the ionization constant of light water proposed by Prof. Peter Tremaine (University of Guelph, Canada) and Dr. Hugues Arcis (NNL, UK) – H. Arcis gave a related presentation during PCAS symposium. New set of high-temperature data for ionization constant of light water has been measured, which is supposed to form a basis for the new formulation. There is a plan to set up a task group in 2023. P. Tremaine gave details about direct conductivity measurements for ionization constant of water, large data database was gathered already showing shortcomings with current formulation, cooperation with S. Lvov is planned. Update on activities will be presented during 2022 meetings.

(3) A joint PCAS/TPWS Task Group to work on developing a guideline on self-diffusion coefficients of H_2O (led by K. Yoshida). This guideline is a work in progress and will continue in the following years.

10. PCAS membership

K. Yoshida proposed the following four researchers as new members of PCAS:

- Tatsuya Ishiyama (University of Toyama, Japan) – 2020 Helmholtz award winner
- Jacy Conrad (Idaho National Laboratory, USA)
- Lucy Platt (National Nuclear Laboratory, UK)
- Chris Alcorn (Los Alamos National Laboratory, USA)

No objections have been raised.

PCAS member Andrey Plyasunov (Russian Academy of Sciences, Russia) asked in July 2021 to be removed from PCAS mailing list.

K. Yoshida will report the changes in PCAS membership to the Executive Committee.

11. Planning activities for 2021/2022

It is still uncertain, whether 2022 meeting in New Zealand will be in-person or on-line. There are several options to tackle limitations on in-person gatherings:

- some parts of the meeting could be held in hybrid style (having in mind different time zones in the EU and USA),
- there could be an option for connecting by videocalls (MS Teams) to certain parts of the meeting (WG meetings),

- on-demand streaming of content on a password-protected service could be available for a certain period of time after the meeting (to make presentations by WG members available for members of other WGs).

P. Tremaine mentioned research activities in geothermal power in New Zealand. This may be an area for broadening PCAS interest.

K. Yoshida mentioned that JPAPWS and NZAPWS hold an online meeting on April 20, 2021. D. Addison, N. Okita, N. Yamaguchi, S. Senoo, S. Terada, and K. Yoshida discussed Geothermal White Paper and Future Possible IAPWS Geothermal Steam TGD. They also discussed technologies for steam scrubbing and improving steam purity.

H. Arcis reported on the activities of Don Palmer concerning an upcoming OECD NEA volume on thermodynamic of ancillary data relevant to nuclear repositories that should soon be published. The elements/compounds treated/evaluated include: boron, phosphorous, aluminum, silica, magnesium, and calcium. A new set of internally consistent, recommended thermodynamic properties of both solid and solution species will be presented. Don Palmer's coauthors are Malcolm Rand, Jean Fugers and Tamas Gadja.

12. Preparation of report for Executive Meeting

K. Yoshida summarized the items that will be reported during 2021 EC meeting (September 17, 2021) – 2021 PCAS symposium, task groups activities, new PCAS members.

The chairman closed the meeting at 13:25 BST.

IAPWS Physical Chemistry of Aqueous Systems (PCAS) Working Group

Agenda 2021

27 August 2021, 12:00− 14:00 (British Summer Time), Online (Teams)

(1) Adoption of agenda

(2) Appointment of clerk of minutes

(3) Approval of minutes from the 2021 meeting
The minutes of 2020 PCAS meetings online (e-mail communication):
http://www.iapws.org/minutes/2020/Minutes2020.pdf

(4) Report of 2021 IAPWS PCAS Symposium, 26 August

(5) Self-introduction and quick reporting on PCAS-related activities (2-3 min each)
- Canada: Prof. Peter Tremaine, Dr. Jane Ferguson
- Japan: Prof. Masaru Nakahara, Prof. Nobuyuki Matubayasi, Dr. Ken Yoshida
- Czech Republic: Dr. Tomáš Němec, Dr. Milan Sedlář, Dr. Ivo Jiricek, Dr. Meenakshi Seshadhri Garapati
- UK: Dr. Hugues Arcis

(6) Possibility of ICRNs
- A few words of explanation from Chair for new PCAS members (http://www.iapws.org/icrn.html)
- Opportunity to discuss expression of interest from PCAS members

(7) International collaboration
- Opportunity to discuss expression of interest from PCAS members

(8) Discussion of PCAS focus – strategy to expand WG
- Open for suggestions regarding approaching other research groups/institutions to gauge potential interest

(9) Discussion of the possibility of releases and guidelines
- A joint PCAS/TPWS Task Group to work on developing a formulation for the static dielectric constant of heavy water is proposed by Dr. Allan Harvey (NIST, USA) and Prof. Peter Tremaine (University of Guelph, Canada). To be created in 2022.
- A joint PCAS/TPWS Task Group to work on developing a formulation for the ionization constant of light water is proposed by Prof. Peter Tremaine (University of Guelph, Canada) and Dr. Hugues Arcis (NNL, UK). To be created in 2023.

- A joint PCAS/TPWS Task Group to work on developing a guideline on self-diffusion coefficients of H_2O (led by K. Yoshida). Development by individual Task Group members is in progress.

(10) PCAS membership

New members:

- Tatsuya Ishiyama (University of Toyama, Japan)
- Jacy Conrad (Idaho National Laboratory, USA)
- Lucy Platt (National Nuclear Laboratory, UK)
- Chris Alcorn (Los Alamos National Laboratory)

Leaving members:

- Andrey Plyasunov (Russian Academy of Sciences, Russia)

(11) Planning activities for 2021/2022

- Progressing ongoing activities.

(12) Preparation of report for Executive Meeting

August 27, 2021
K. Yoshida (Chair)
H. Arcis (Vice Chair)

The International Association for the Properties of Water and Steam

Power Cycle Chemistry Working Group (PCC WG)

VIRTUAL WEBMEETING – 31 August 2021

10:00 – 12:00 (Swiss Time) – PCC WG Meeting

Welcome from Michael to the Virtual PCC Meeting in these difficult times and thanks to everyone across all the time zones.

1. Amendments / Adoption of Agenda (Attachment 1)

   Accepted

2. Appointment of Clerk of Minutes

   David Addison - NZAPWS

3. Review of Actions from last PCC WG Meeting
   - PCC members need to check action items from 2019 minutes and provide a short and brief status on summary of actions from PCC 2019
   - Email please directly to PCC Chairmen Addison & Rziha latest by 17th September.
     List of action items is here attached (Attachment 2)

4. Actual Status of IAPWS TGD's – (Barry Dooley, et. al.)

   Barry has contacted all TGD working group members to get a status update for them all. The status is divided into three categories

   - Those that are **active**
   - Those that are **static** and not moving ahead – need to decide to keep ahead or retire.
   - Those that are **new** and need to be decided as to they move ahead

   1. **ACTIVE**
      Geothermal (white paper)

      Been discussed with the Japanese IAPWS and geothermal power plant OEMs – comments from initial draft together, need to do a re-write based on their feedback – currently sitting with Addison/Richardson (NZAPWS).

Then more discussions with Japanese and then circulation to wider IAPWS PCC and outside to geothermal etc and then move to full TGD.

White Paper "Corrosion Product Sampling, Monitoring for Flexible and Fast Starting Plants"

White paper presented in Banff 2019. Sent out to review by PCC and by Barry to others around the world – USA chemists, HRSG forums etc. Some good feedback on the decay map, offers to share data etc. Taking these comments to produce a final draft of the white paper. Data only includes good plants with optimal chemistry. Looking for some "suboptimal plants" to get some more data for the decay map. Applied in Banff for a IC – for $20,000 pounds for a student to do some work – currently on hold due to COVID. Need to sort out how to move forward in current environment. Need more data to validate concept.

Water Treatment of Flue Gas Condensate White Paper

Monika Nielsen to take the lead on the TGD. White paper delayed. Working group being re-started. Working draft. Target beginning of 2022 for PCC circulation.

Electrode Boilers

Information sharing between NZAPWS and SIAPWS going well. Good learnings and support between both groups. Vendors very chemistry uninformed. Moving to produce some technical papers to get more information out there, case studies etc and then look at a white paper and possible section for current TGDs or a new TGD. In progress.

2. **STATIC**:

Nuclear FFS Possible TGD

Work started in 2017 to develop a white paper. Group estimated at Banff 2019, rough outline worked up. Original target for initial draft in 2020. Missed target, limited work done to date.
Joerg Fandrich has offered to take over chair of this working group to develop a draft by end of the year. Has Framatome support and budget to do this.
Action: Barry to get this change made and to be involved as well.

3. **RETIRE**
   Demin Water Integrity

First discussed in Boulder in 2012, oldest TGD in development. First incomplete draft in June 2014. Nothing else really happened since then.
Decision: This TGD will be retired until further notice.

Condensate Polishers

First discussed in 2018, minimal progress to date. Moataz would like to continue with TGD if possible. Some initial writing was done.
Barry – suggests to leave it for a year.
Decision: Re-evaluation and final decision in 2022

Smart Alarms

First discussed in Banff 2019. Thought it could be added to the instrumentation TGD as an appendix.
Rough draft done in 2020 and circulated to PCC. Based on feedback received from PCC WG some thoughts / comments:

- Possible mistake to try to combine with Instrumentation TGD – dilutes the usefulness of the current TGD
- Becoming a commercial issue with more specific direction of analyser technology
- Smart Alarms are a "licenced product" from EPRI which makes incorporation in a TGD challenging.

➔ Suggest that smart alarms get retired but the instrumentation TGD gets a possible revision / amendment. No objection from the WG, hence this amendment will be prepared for the annual meeting in 2022.

4. Advisory note for Oil Recovery Systems – taking relevant information from current TGDs for this.

   First discussed at Banff 2019. No progress since then.

5. Proposals for new TGD's

   None at this stage.

6. Revisions of current TGDs?

   Some minor updates needed to a few, correction of errors etc. Can be done at anytime if people feel it needs doing.
   Can be done and circulated to PCC for comment and then approval at next IAPWS annual meeting. Any suggestions, notes, etc. should be send to both chairmen and Barry Dooley.

PCC WG Business:

1. **International Collaboration**

- Boiler Corrosion – Canada/NZ – work continuing but no visits due to COVID.
- Additional EPRI funding for extending the research obtained. Goal to so have papers published at some time.

- No additional IC projects suggested at this stage

2. ICRNs – Review and Possible New Additions

- Suggestion by Addison – ICRN for superheated steam and FFS interactions.
  To be drafted for next IAPWS meeting. Presentation to be made to IAPWS virtual symposium to help identify the areas that are deficient in the science of FFS to date (Dooley/Addison) – major deficiency is knowledge about what happens to the oxide growth in feedwater/boiler/steam with a FFS present. Discussions held with PCAS – doing work on supercritical oxidation, keen to do more research in this area.

3. Changes in PCC Membership and Election of Officers

Following persons have expressed their wish becoming a member of IAPWS PCC:

- Mr. Herman Kempen, Kurita Germany (absent)
- Mr. Hal Stansfield, Waltron USA (absent)
- Mr. Jon Guy, Waltron USA (absent)
- Dr. Hugues Arcis, National Nuclear Laboratory Limited UK (**present**)
- Mrs. Lucy Platts, National Nuclear Laboratory Limited UK (**present**)
- Mrs. Maria del Mar Nogales Lopez, SWAN AG, Switzerland (**present**)

Michael supports the membership of Hugues, Lucy and Mar (those in attendance) to the PCC.
Barry – Seconded for their membership.
Those being unable to attend this meeting will be kept in the loop of information from PCC and may be proposed officially as member during the next annual meeting, when present.
No objections raised – **ACCEPTED**

ACTION:

Michael will propose these 3 persons to the EC, becoming an official member

4. **Change in PCC Chairmanship**

- David Addison suggested to take over from Michael at the IAPWS upcoming EC meeting. This is supported by PCC. Barry supports this – suggests that Michael stays on as vice chair for a year for continuity and support. Michael agreed.
- PCC WG accepted David as new chairman unanimously.
- Barry would like to say thank you for the excellent and dedicated work to IAPWS and PCC from Michael for over the last 10 years

5. Adjournment

Michael expressed his appreciation to all present, participating in this virtual meeting, despite the harsh circumstances for many participants, caused by the wide variation of time zones.

Meeting was closed.

Power Cycle Chemistry Working Group (PCC WG)

VIRTUAL WEBMEETING Agenda

10:00 – 12:00 (Swiss Time) – PCC WG Meeting

a) Amendments / Adoption of Agenda

b) Appointment of Clerk of Minutes

c) Review of Actions from last PCC WG Meeting

d) Actual Status of IAPWS TGD's – (Barry Dooley, et. al.)

1) Geothermal (white paper)
2) Smart Alarms
3) White Paper
   " Corrosion Product Sampling, Monitoring for Flexible and Fast Starting Plants"
4) Water Treatment of Flue Gas Condensate White Paper
5) Other open TGD (Cond. Pol., Demin Plant)
6) Proposals for new TGD's

PCC WG Business:

a) International Collaboration

b) ICRNs – Review and Possible New Additions

c) Changes in PCC Membership and Election of Officers

d) Adjournment

IAPWS Canadian National Committee

Annual Report 2021

Submitted to IAPWS EC, Virtual Meeting, September 17, 2021

CNC Executive: *William Cook (Chair); Glenn Pringle (COG – adhering organisation), Derek Lister; Peter Tremaine; Melonie Myszczyszyn; Rich Pawlowicz; Craig Stuart; Olga Palazhchenko; Sarita Weerakul, Jane Ferguson*

1. Canadian National Committee: Dues for the Canadian National Committee (CNC) of IAPWS are supported by the National Research Council (NRC) of Canada. This arrangement requires support and participation by a national organization representing industry. The agreement with the CANDU Owners Group (COG) and the NRC on its third five-year term expired in June 2021 and is currently being renewed for another five-year period.

2. CNC Activities

Due to the COVID-19 global pandemic, the CNC, as a whole, has had minimal activities over the past year. Individual's continuing activities over the past year are highlighted below.

2.2 Activities at the University of New Brunswick (UNB)

Derek Lister

During the last year or so, UNB Nuclear's major activities relating to IAPWS have been as follows:

- Investigating the effects of a film-forming amine on the flow-accelerated corrosion of carbon steel under two-phase feedwater conditions; the influences of temperature, steam quality and flow have been measured.
- Developing a technique for measuring the streaming potential of corrosion-product particles under reactor primary coolant conditions; zeta potential values have been derived and are being incorporated into a model for particle transport.
- Demonstrating the effects of gamma radiation on the corrosion of printed aluminum components in seawater; printed components corrode less than normal cast components and cobalt-60 irradiation exacerbates the attack.
- Evaluating the effects of a dispersant on the flow-accelerated corrosion of carbon steel under power plant feedwater conditions.
- Determining the mechanisms of aluminum alloy corrosion and corrosion-product release under conditions of a loss-of-coolant accident in reactor containment.
- Modelling the diffusion of hydrogen through steel to support the development of CNER's HePro for measuring the flow-accelerated corrosion of power plant piping.
- Investigating the suitability of a film-forming amine for inhibiting secondary-side corrosion during reactor lay-up.

These studies involve collaboration with the French CEA at their Cadarache facility and support from, among others, Kurita Water Industries in Japan, Framatome in Germany and EPRI in the

US.

Willy Cook

As Director of UNB's CNER Institute (Centre for Nuclear Energy Research), W. Cook continues to expand CNER's consulting expertise and services to Canada's nuclear industry. Activities include engagement with local nuclear power generating stations and the Canadian Nuclear Laboratories, the Candu Owners Group and other utilities.

In 2018, CNER partnered with the provincial government and several advanced nuclear reactor designers and vendors with the intention of establishing a Small Modular Reactor Research Cluster within the Province. This has led to a significant expansion of activities at the research institute including continuing work of interest to IAPWS and the PCC working group.

CNER's HEPro corrosion monitoring has made the next step to commercialization with installation at another nuclear plant and several planned installations on both Primary Heat Transport System components and in the Secondary System, targeted at final feedwater and reheater drains return locations. Several COG programs are continuing, and these activities are being supported through a growing partnership between UNB-CNER and the Canadian Nuclear Laboratories.

The IC project that W. Cook and D. Addison (Thermal Chemistry Inc. – New Zealand) completed the first phase for several years ago has been continuing with support from EPRI. The focus of the project is to measure, electrochemically, the effects of mixed contaminants on boiler materials to support the current contaminant concentration specification and action levels.

Olga Palazhchenko

In March 2021, Olga transitioned from a Research Associate working at UNB-CNER to an Assistant Professor within UNB's Department of Chemical Engineering. Her activities of interest to IAPWS include:

- Incorporation of the new D_2O formulations for various thermochemical properties into the boiler heat transport code at UNB-CNER as part of a project to model RIHT rise in CANDU plants. This resulted in two recent publications in the PPCHEM journal.
- Collaborative COG project with CNL on ion exchange resin aging and hydrolysis, which has continued on as an independent project at CNER.
- Collaboration with CNL to deliver a virtual CANDU Chemistry course to over 60 participants in 2020 and another follow up course this upcoming October.
- On going benchmarking of modelled magnetite deposits to station data with support from PLNGS.

2.3. Activities at the University of Guelph (Peter Tremaine)

The NSERC/UNENE Senior Industrial Research Chair in High Temperature Aqueous Chemistry was awarded to Professor Peter Tremaine at the University of Guelph in 2016 and is currently undergoing renewal for another five-year term. As part of the previous term, a new Associate Professor was hired as the Jr. Research Chair – Prof. Kash Ghandi.

The purpose of the Chair is to expand mission-oriented basic research and modelling expertise in

areas related to the primary coolant chemistry, moderator chemistry, and steam-generator chemistry of the CANDU reactor fleet, as well as in areas related to the geological storage of nuclear spent fuel. The funding model is new for a UNENE IRC, in that support has been provided by three other industrial partners, in addition to UNENE: the CANDU Owner's Group (COG), the Nuclear Waste Management Organization (NWMO) and the Electric Power Research Institute (EPRI). Recent activities include:

- Membership in the EPRI MULTEQ Database Advisory Committee.
- Dr. Tremaine and Dr. Andrej Skerencak-Frech (Karlsruhe Institute of Technology) have been invited by the NEA to prepare an Initiation Report for the NEA/OECD Thermodynamic Database Project, making the case for a State-of-the-Art Report on modelling the effects of temperature and pressure on chemical equilibria under spent-fuel geological storage conditions.
- A collaborative project with the US National Institute of Standards and Technology (NIST) has been initiated to develop formulations for the dielectric constant of heavy water up to CANDU primary coolant operating temperatures. None exist at this time.

2.4. Activities at the University of British Columbia (Rich Pawlowicz)

No updates received, Dr. Pawlowicz conducting field work.

2.5. CANDU Owner's Group (COG) Activities

COG is a not-for-profit corporation with voluntary funding from international CANDU-owning utilities and Canadian National Laboratories. The COG mission is to improve the performance of CANDU stations worldwide through member collaboration. COG Canadian R&D program members include Ontario Power Generation, Bruce Power Limited Partnership, New Brunswick Power and Canadian Nuclear Laboratories.

CANDU Industry-IAPWS Engagement
Craig Stuart (CNL) is a member of the COG Technical Committee for CM&C. Willy Cook and Peter Tremaine have participated in the Chemistry Working Group meetings and other COG workshops and have also provided input to the annual COG R&D planning process. W. Cook keeps the Working Group members informed of the Canadian IAPWS activities.

COG was the primary sponsor for the CNC when we hosted the 2019 IAPWS Annual Meeting and continue to be our adhering organization in partnership with the National Research Council (NRC) who pay the CNC's dues to the association.

2.6 Oil Industry Activities

No updates received.

4. Activities Planned

The CNC activities over the next few years will continue the work that is currently ongoing, as described above. With the uncertainty of when restrictions will be lifted during the pandemic,

no significant CNC activities are currently being planned.

5. Select List of Publications

Published and Submitted Research Papers (2020-2021)

1. M. Yacyshyn, L. Applegarth, J. Cox and P. Tremaine. Deuterium Isotope Effects on the Second Ionization Constant of Aqueous Sulfuric Acid from 25 °C to 200 °C using Raman Spectroscopy. *J. Solution Chem*. (Submitted)
2. S. Binkley, O. Fandino, J.S. Cox and P. Tremaine, Standard Partial Molar Heat Capacities and Volumes of Aqueous N,N-Dimethylethanolamine (DMEA) and N,NDimethylethanolammonium Chloride from 283.15 K to 393.15 K, and Ionization Constants to 598.15 K, *J. Chem. Eng. Data.* (Submitted)
3. Conrad, J; Tremaine, P. Third Dissociation Constant of Phosphoric Acid in H_2O and D_2O from 75 to 300 °C at p = 20 MPa using Raman Spectroscopy and a Titanium-Sapphire Flow Cell. *Phys. Chem. Chem. Phys*. **23**, 10670 – 10685 (2021).
4. Fandino Torres, O; Cox, J; McGregor, C*; Conrad, J*; Liao, K; Tremaine, P. Carbon Dioxide Contamination of Aqueous Morpholine Solutions and Effects on Secondary Coolant Chemistry under CANDU Conditions. *Nuclear Technology*. (2021). On-line Journal.
   DOI: https://doi.org/10.1080/00295450.2020.1862471
5. H. Arcis, J.P. Ferguson, J.S. Cox, P.R. Tremaine. The Ionization Constant of Water at Elevated Temperatures and Pressures: New Data from Direct Conductivity Measurements and Revised Formulations from T = 273 K to 674 K and p = 0.1 MPa to 31 MPa. *J. Phys. Chem. Ref. Data*. **49**(3): 033103-1 to 33103-37 (2020). **Selected as "Editors' Pick"**
6. J. Conrad, S. Sasidharanpillai, P.R. Tremaine, The Second Dissociation Constant of Carbonic Acid in H_2O and D_2O from 150 to 325 °C at p = 21 MPa using Raman Spectroscopy and a Sapphire-Windowed Flow Cell. *J. Phys. Chem. B,* **124**(13): 2600-2617 (2020).
7. Cherpin, D. Lister, F. Dacquait and L. Liu. Study of the Solid-State Synthesis of Nickel Ferrite (NiFe2O4) by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Raman Spectroscopy. *Materials*. 2021; 14(10):2557. https://doi.org/10.3390/ma14102557.
8. D. Lister. Materials of the Heavy-Water Systems of CANDU Reactors. Techniques de l'Ingénieur. In press - 2021.
9. S. Weerakul, N. Leaukosol, D.H. Lister, S. Mori and W. Hater. Effects on Flow-Accelerated Corrosion of Oleylpropanediamine Under Single-Phase Water Conditions Pertinent to Power Plant Feedwater. CORROSIONJOURNAL.ORG. Vol. 76, Iss. 2, P. 217. 2020 February.
10. J. Huang, D. Lister and S. Uchida. The Corrosion of Aluminum Alloy and Release of Hydrogen in Nuclear Reactor Emergency Core Coolant: Implications for Deflagration and Explosion Risk. Nuclear Engineering and Design. 359 (2020) 110458.
11. Palazhchenko, O; Cook, W; Martin, A; Lennox, J. (2021). Update on Predicting RIHT Using the UNB-CNER CANDU-6 PHT System Model. PowerPlant Chemistry. 23(3): 122-131.
12. Palazhchenko, O; Cook, W; Martin, A; Taylor, D. (2020). Heat Transfer Add-on to the UNB-CNER CANDU-6 PHT System Material Transport Model. PowerPlant Chemistry. 22(6): 262-273.

Technical Reports

1. Carbon Dioxide Contamination of Aqueous Morpholine Solutions and Effects on Secondary Coolant Chemistry under CANDU Operating and Start-up Conditions, COG Report OP-18-4075 (CANDU Owners Group Project: WP 40194, 2018-2020)
2. Chemistry Aspects of Hot Conditioning during Darlington 2 Return to Service, Kinectrics Report to OPG, P. Spekkens, D. Evans, D. Guzonas, P. Tremaine (Finalized March 2020)
3. D. Lister, A. Turner and S. Weerakul. Effect of Oxide Dissolution on Material Transport in Reactor Coolant Systems. Coolant Chemistry Control and Effects on Fuel Reliability in Pressurized Heavy Water Reactors – Report of a Technical Meeting. IAEA-TECDOC-1942. International Atomic Energy Agency, VIENNA, 2021.
4. W.G. Cook, E. Saulnier, B.J. McCann and C.R. Stuart, Hydrogen Effusion Measurements Update 2019-2020 – Operation under Steam Cycle Conditions, COG Report OP-19-4058 (COG CM&C WP 40751)
5. C.R. Stuart, J.A. Gauthier, O.Y. Palazhchenko and W.G. Cook, The Influence of the PHTS Purification System on Iron Transport and Feeder Integrity, COG Report COG-19-4003 (COG CM&C WP 40186)
6. O.Y. Palazhchenko, W. Cook, J. Ferguson and C.R. Stuart, Lithium Removal on Aged IX Resins and Outage pHa Depression, COG Report COG-20-4009 (COG CM&C WP 40199)
7. D.S. Mancey and W.G. Cook, State-Of-The-Art Report on Flow-Accelerated Corrosion, COG Report COG-17-4051 (COG CM&C WP 40741)

Published Proceedings from Conferences and Workshops

1. P. Tremaine, J. Conrad, H. Arcis, J. Cox (2020) Chemical Modelling Studies of Magnetite Solubility Effects During CANDU Reactor Start-Up and Hot Conditioning, in International Atomic Energy Agency IAEA-TECDOC-1942IAEA-TECDOC-1942, Report of a Technical Meeting on the Control and Monitoring of Coolant Chemistry and Related Issues on Fuel Reliability in Pressurized Heavy Water Reactors (Sponsored by COG & CNSC, Toronto, Canada, Nov. 25-27, 2019).
2. S. Weerakul, N. Leaukosol, D. Lister, S. Mori and W. Hater. Exploring the Effects of the OLDA Product G851® on the FAC of Carbon Steel Under Two-Phase Feedwater Conditions. Proc. IAPWS Fourth International Conference on Film Forming Substances (FFS2021). Virtual, 2021 March 23-25.
3. N. Leaukosol, S. Weerakul and D. H. Lister. In-loop Tests of Probe for Flow-accelerated Corrosion Monitoring in Power-plant Feedwater. Proc. 41st Annual Conference of Canadian Nuclear Society & 45th Annual CNS/CNA Student Conference. Virtual, 2021 June 6-9.
4. S. Raval, R. Trivedi and D. Lister. Machine Learning Techniques to Predict Flow Accelerated Corrosion Rate and Scalloping Behavior. Proc. SAIMIN 2020: 1st Symposium on Artificial Intelligence, Machine Learning and Other Innovative Technologies in Nuclear Industry. Canadian Nuclear Society. 2020 October.
5. J.A. Flood, W.G. Cook, F. Zeuchner, N. Sawyer, Casting and Production of HT9 for Advanced Reactor Fuel Cladding, Proc. 40th Annual Conference of Canadian Nuclear Society & 44th Annual CNS/CNA Student Conference. Virtual, 2020 June.
6. J. Kongtuk and W. Cook, Investigation of the Impacts of Octadecylamine (ODA) and

Cyclohexylamine (CHA) on Ion Exchange Capacity and Mass Transfer Coefficient (MTC), Proc. 41st Annual Conference of Canadian Nuclear Society & 45th Annual CNS/CNA Student Conference. Virtual, 2021 June.

Czech Society for the Properties of Water and Steam

Annual Report 2021

Submitted to IAPWS Executive Committee, September 2021

Steering board of CZPWS

Chair: Tomáš Němec (Institute of Thermomechanics of the Czech Academy of Sciences - IT CAS, nemec@it.cas.cz), Vice-Chair: Josef Šedlbauer (Technical University of Liberec), Secretary: Jan Hrubý (IT CAS), Member: Radim Mareš (University of West Bohemia), Member: Milan Sedlář (SIGMA Research and Development Institute).

CZPWS Meetings

Annual meeting of the CZPWS was held on June 23, 2021. Due to the covid-19 situation, the form of the meeting was electronic. CZPWS members were informed about the activities of CZPWS Chair and approved CZPWS Financial Statements. The 2021 payment of CZPWS Member Due to IAPWS was provided from a national grant led by T. Němec. In 2021, CZPWS became a member of the Council of Scientific Societies of the Czech Republic (CSSCR). Future CZPWS Member Dues to IAPWS will be paid based on the CZPWS membership in CSSCR. The process of enrolling CZPWS into CSSCR was long and required significant efforts primarily from the side of CZPWS Chair.

RESEARCH ACTIVITES

Surface tension of aqueous systems

Experimentalists from IT CAS in Prague continued an investigation of the surface tension of aqueous systems at low temperatures, including the supercooled metastable state. Preliminary data for the surface tension of water + ethylene glycol were presented at the 21st Symposium on Thermophysical Properties held in Boulder (USA) in June 2021 [10]. The team also developed own calibration technique based on the work of Fritz et al. [J. Phys. Chem. B 104 (2000) 15] for a highly sensitive commercial instrument – the vibrating tube densimeter Anton Paar DMA 5000 M. The results for air + water calibration and a series of reference liquids with various viscosities were also presented at the Boulder conference [11] and are being prepared for a journal publication.

Recent work on surface tension of supercooled water at University of West Bohemia in Pilsen was reported by R. Mareš and J. Kalová [1].

Nucleation and condensation

M. Šťastný (University of West Bohemia in Pilsen) published a broad review of steam condensation in nozzles and turbines a form of a book chapter [2] and a textbook [3].

J. Hrubý (IT CAS) participated in the research of nucleation of droplets in the water – sulfuric acid system [4]. In collaboration with group of V. Ždímal (Institute of Chemical Process Fundamentals of

the Czech Acad. Sci.), a new device was developed and the corresponding mathematical models were tested. J. Hrubý continued in the research of the effect of carrier gases on nucleation of water droplets in collaboration with group of D. Smeulders (Eindhoven University of Technology, Netherlands). Recent work focused on water nucleation in mixtures with carbon dioxide and nitrogen at various mixing ratios and various pressures [5].

Cavitation

The problems studied in the SIGMA Research and Development Institute and the Centre of Hydraulic Research in the period of June 2020 – June 2021 have been related mainly to the modelling of cavitation erosion during the hydrodynamic cavitation and models of cavitation instabilities. In cooperation with the Institute of Physics of the Czech Acad. Sci., a new cavitation erosion stand has been put into operation. In cooperation with the Moscow Power Engineering Institute, the Technical University of Liberec and the Wuhan University, the experimental and numerical modelling of unsteady cavitation phenomena in water has continued in the framework of internal grant projects. The experiments and numerical simulations have concentrated on the thermal effects of cavitation and on the influence of surface hydrophobicity on cavitation phenomena [6]. In cooperation with IT CAS and the Technical University of Ostrava, the experimental and numerical modelling of unsteady multiphase flow has continued, taking into account the interface of water and air [7].

Other work

A. Blahut (IT CAS) served in an evaluation task group in the evaluation of proposed IAPWS formulations on the viscosity of heavy water [(IAPWS R17-20, Release on the IAPWS Formulation 2020 for the Viscosity of Heavy Water (2020)] and on thermal conductivity of heavy water [IAPWS R18-21, Release on the IAPWS Formulation 2021 for the Thermal Conductivity of Heavy Water (2021)].

Publications

1. Kalová J., Mareš R.: Surface Tension in the Supercooled Ware Region, Int. J. of Thermophysics 42 (2021) 131.

2. Šťastný M.: New Ideas Concerning Science and Technology, Vol.4, Chapter 1, Investigation on Losses Connected with Steam Condensation in Turbine Cascades, Book Publisher International, India+United Kingdom, 2021, ISBN 978-81-949988-9-1.

3. Šťastný M.: Condensation of Steam in Nozzles and Turbine Cascades. ZČU, Fakulta strojní, Plzeň, 2015, ISBN 978-80-261-0489-6.

4. Trávníčková T., Havlica J., Kozakovic M., Hrubý J., Ždímal V.: Derivation and validation of a simplified analytical mass transref model of the laminar co-flow tube for nucleation studies. Int. J. Heat and Mass Transfer 179 (2021) 121705. https://doi.org/10.1016/j.ijheatmasstransfer.2021.121705

5. Campagna M.M., Hrubý J., van Dongen M. E. H., and Smeulders D. M. J.: Homogeneous water nucleation in carbon dioxide – nitrogen mixtures: Experimental study on pressure and carrier

gas effects. J. Chem. Phys. 154 (2021) 154301 https://doi.org/10.1063/5.0044898

6. Sedlář M., Komárek M., Šoukal J., Volkov A.V., Ryzhenkov A.V., Naumov A.V., Druzhinin A.A., Vikhlyantsev A.A.: Experimental and Numerical Investigation of Impacts of Cavitation on Hydrofoils with Treated Surfaces. Thermal Engineering, submitted June 2021
7. Sedlář M., Machalka J., Komárek M.: Modeling and Optimization of Multiphase Flow in Pump Station. Journal of Physics, 1584 (2020), 012070. doi:10.1088/1742-6596/1584/1/012070
8. Sedlář M., Procházka P., Komárek M., Uruba V., Skála V.: Experimental Research and Numerical Analysis of Flow Phenomena in Discharge Object with Siphon. Water 12 (2020) 3330. doi:10.3390/w12123330
9. Furst J., Halada T., Sedlář M., Krátký T., Procházka P., Komárek M.: Numerical analysis of flow phenomena in discharge object with siphon using lattice-Boltzmann method and CFD. Mathematics, submitted June 2021

Conference Proceedings

10. Vinš V., Hykl J., Prokopová O., Gatter J., Klomfar J., Součková M., Čenský M., Blahut A.: Surface tension and density of water + ethylene glycol mixtures at low temperatures including metastable supercooled state, 21st Symposium on Thermophysical Properties, Boulder, Colorado, 20-25 June 2021.
11. Prokopová O., Blahut A., Čenský M., Součková M., Vinš V.: Water & air calibration of vibrating-tube densimeter at temperatures from 0 to 90 °C and atmospheric pressure. 21st Symposium on Thermophysical Properties, Boulder, Colorado, 20-25 June 2021.

German National Committee to IAPWS Executive Committee

Research Activities on the Thermodynamic Properties of Water and Steam of the German National Committee and of Partners in Switzerland in the Period 2020/2021

www.iapws.de

Chair: Prof. Dr. Hans-Joachim Kretzschmar
Zittau/Goerlitz University of Applied Sciences, Zittau

Vice Chair: Ingo Weber
Spardorf

Annual Meeting of the German National Committee

The Annual Meeting of the German National Committee was planned at the GFZ German Research Centre for Geosciences in Potsdam for March 2021, but had to be canceled due to Corona situation.

In the following, activities of certain members of the German National Committee are summarized.

Baltic Sea Research Institute, Warnemuende
Dr. Rainer Feistel

Recent Publications

- Ebeling, W., Feistel, R., Camoes, M.F.:
  Trends in statistical calculations of individual ionic activity coefficients of aqueous electrolytes and seawater.
  Trends in Physical Chemistry (2020), 20:1-26
  http://www.researchtrends.net/tia/abstract.asp?in=0&vn=20&tid=16&aid=6609&pub=2020&type=3
- Weinreben, S., Feistel, R.:
  Anomalous salinity-density relations of seawater in the eastern central Atlantic.
  Deep–Sea Research I 154 (2019) 103160, https://doi.org/10.1016/j.dsr.2019.103160
- Feistel, R.:
  Distinguishing between Clausius, Boltzmann and Pauling Entropies of Frozen Non-equilibrium States.
  Entropy 2019, 21(8), 799; https://doi.org/10.3390/e21080799
  (Editor's Choice article)
- Hellmuth, O., Schmelzer, J.W.P., Feistel, R.:
  Ice-Crystal Nucleation in Water: Thermodynamic Driving Force and Surface Tension. Part I: Theoretical Foundation.
  Entropy 2020, 22(1), 50; https://doi.org/10.3390/e22010050
- Feistel, R., Hellmuth, O.:
  Zur Rolle des Wassers in der Energiebilanz des Klimasystems.
  Sitzungsberichte der Leibniz-Sozietät der Wissenschaften zu Berlin 144 (2020) 51-139,

https://leibnizsozietaet.de/publikationen/sitzungsberichte/

English translation:
On the Role of Water in the Energy Balance of the Climate System,
https://doi.org/10.13140/RG.2.2.19649.17766

- Hellmuth, O., Feistel, R.:
  Analytical Determination of the Nucleation-Prone, Low-Density Fraction of Subcooled Water.
  Entropy 2020, 22(9), 933; https://doi.org/10.3390/e22090933
- Ebeling, W.; Feistel, R.; Krienke, H.:
  On statistical calculations of individual ionic activity coefficients of electrolytes and seawater. I.
  Online preprint 14 Apr 2019.
  DOI: 10.13140/RG.2.2.18591.20640
- Feistel, R.:
  Defining relative humidity in terms of water activity. Part 2: relations to osmotic pressures.
  Metrologia 56, 015015 (2019).
  https://doi.org/10.1088/1681-7575/aaf446
- Hellmuth, O.; Shchekin, A. K.; Feistel, R.; Schmelzer, J. W. P.; Abyzov, A. S.:
  Physical interpretation of ice contact angles, fitted to experimental data on immersion freezing of kaolinite particles.
  Interface. Phenom. Heat Transfer 6, 37-74 (2018).
  DOI: 10.1615/InterfacPhenomHeatTransfer.2018026166
- Hellmuth, O., Feistel, R.; Foken, T.:
  Intercomparison of Different State-of-the-Art Formulations of the Mass Density of Humid Air.
  Bull. Atmos. Sci. Tech. (2021), in press, https://doi.org/10.1007/s42865-021-00036-7
- Feistel, R.:
  Thermodynamic Properties of Seawater, Ice and Humid Air: TEOS-10, Before and Beyond.
  Ocean Sci. 14, 471-502 (2018).
  https://doi.org/10.5194/os-14-471-2018
- Burchard, H.; Bolding, K.; Feistel, R.; Gräwe, U.; Klingbeil, K.; MacCready, P.; Mohrholz, V.; Umlauf, L.; van der Lee, E.:
  The Knudsen theorem and the Total Exchange Flow analysis framework applied to the Baltic Sea.
  Progress in Oceanography 165, 268-286 (2018).
  https://doi.org/10.1016/j.pocean.2018.04.004
- Feistel, R.; Lovell-Smith, J. W.:
  Implementing systematic error in the weight matrix of generalized least-squares regression.
  published online (2018).
  https://doi.org/10.13140/RG.2.2.25098.16320

Helmut Schmidt University / University of the Federal Armed Forces Hamburg
Institute of Thermodynamics
Prof. Dr. Karsten Meier, Dr. Robert Hellmann

Projects

1. Thermophysical properties of mixtures of water vapor and simple gases from first-principles calculations.

2. Measurements of the speed of sound in water and derived thermodynamic properties of water.

Recent Publications

- Hellmann, R.; Harvey, A. H.:
  First-Principles Diffusivity Ratios for Atmospheric Isotope Fractionation on Mars and Titan
  J. Geophys. Res. Planets 126, e2021JE006857 (2021).
- El Hawary, A.; Meier, K.:
  Highly Accurate Densities and Isobaric and Isochoric Heat Capacities of Compressed Liquid Water Derived from New Speed-of-Sound Measurements.
  N.N. (2021), in preparation.

Leibniz Institute for Tropospheric Research, Leipzig
Dr. Olaf Hellmuth

Recent Publications (published, in press, submitted, in preparation)

- Foken, T.; Hellmuth, O.; Huwe, B.; Sonntag, D.:
  Chapter 5: Physical Quantities. In: Foken, T. (Ed.): Springer Handbook of Atmospheric Measurements.
  Springer International Publishing. Hardcover, ISBN 978-3-030-52170-7, DOI 10.1007/978-3-030-52171-4 (book chapter). In press.
- Görner, C.; Franke, J.; Kronenberg, R.; Hellmuth, O.; Bernhofer, C.:
  Multivariate non-parametric Euclidean distance model for hourly disaggregation of daily climate data.
  Theoretical and Applied Climatology, 143, pp. 241-265, https://doi.org/10.1007/s00704-020-03426-7 (journal article).
- Hellmuth, O.; Feistel, R.; Foken, T.:
  Intercomparison of different state-of-the-art formulations of the mass density of humid air.
  Bulletin of Atmospheric Science and Technology.
  Bull. Atmos. Sci. Tech. doi:10.1007/s42865-021-00036-7 (journal article).
- Sonntag, D.; Foken, T.; Vömel, H.; Hellmuth, O.:
  Chapter 8: Humidity Sensors. In: Foken, T. (Ed.): Springer Handbook of Atmospheric Measurements.
  Springer International Publishing. Hardcover ISBN 978-3-030-52170-7, DOI 10.1007/978-3-030-52171-4, in (book chapter). In press.
  - Spänkuch, D., O. Hellmuth, U. Görsdorf: What is a cloud? Toward a more precise definition? Bull. Am. Met. Soc. (journal article). In Revision
- Feistel, R., F., Hellmuth, O.:
  Zur Rolle des Wassers in der Energiebilanz des Klimasystems. In: Pfaff, G., R. O. Greiling, R. Pail: Klimawandel – Anzeichen, Ursachen, Folgen.
  Kolloquium der Leibniz-Sozietät der Wissenschaften zu Berlin am 13.2.2020 in der Humboldt-Universität Berlin. Sitzungsberichte der Leibniz-Sozietät der Wissenschaften, Band 144, 51-139, https://leibnizsozietaet.de/wp-content/uploads/2021/03/Gesamtdatei-SB-144-2020.pdf (book chapter).
- Feistel, R., F., Hellmuth, O.:
  On the Role of Water in the Energy Balance of the Climate System.
  Vortrag am 13. Feb. 2020, Kolloquium „Klimawandel – Anzeichen, Ursachen, Folgen“. Leibniz-

Sozietät der Wissenschaften zu Berlin e.V., ResearchGate, https://doi.org/10.13140/RG.2.2.36390.88649 (conference contribution).

- Hellmuth, O., Feistel, R.: Analytical determination of the nucleation-prone, low-density fraction of subcooled water. Entropy 2020, 22(9), 933, https://doi.org/10.3390/e22090933 (journal article)

PPCHEM AG, Hinwil - Switzerland
Michael Rziha

Following Documents are presently in elaboration:

- Chemistry in Geothermal plants (White Paper)
- Corrosion Product Sampling, Monitoring for Flexible and Fast Starting Plants (White Paper)
- Water Treatment of Flue Gas Condensate White Paper
- Chemistry for Electrode Boilers (White Paper)
- FFS application in Nuclear Plants (White paper)
- Demin Water Integrity
- Condensate Polishing Plants
- Smart Alarms

Due to the well-known pandemic situation in 2020 and 2021 the progress of these documents was hampered.

Nevertheless, several documents were progressing well, while some others did not progress for different reasons at all.

Based on this individual status, initial feedback from the PCC WG and the progress forecast it was decided by PCC to divide the individual documents, respectively its status into 3 groups, namely:

- Active
- Static - Retired
- New

Consequently, it was jointly agreed to "retire" the TGD "Demin. Water Integrity", as there was no significant progress during the last 5 years.

The elaboration of the TGD "Smart Alarms" became also retired, since several aspects (e. g. legal issues, as the term "Smart Alarms" is licensed by EPRI) are clearly speaking against such an individual TGD. It was jointly agreed to prepare an amendment to the existing IAPWS TGD2-09(2015) "Instrumentation", covering this topic accordingly and in an appropriate manner.

TGD Condensate Polishing Plants will be kept alive until 2022. In case of there is no significant progress visible until 2022, its retirement will be likely and will be decided during the annual meeting in 2022.

All other documents, as listed here before, will remain active.

PTB German National Metrology Institute
Working Group 3.13, Electrochemistry
Dr. Steffen Seitz

Projects:

1. The working group 3.13 'Electrochemistry' of PTB is part of the European metrology research project "SApHTIES". The project aims to improve the traceability of pHT measurements of seawater, a quantity needed to monitor ocean acidification due to anthropogenic CO2 emissions. Empirical

equations with associated uncertainties will be developed describing pHT in dependence of salinity and temperature over ranges relevant in oceanography.

2. Furthermore, working group 3.13 is associated with SCOR Working Group 145. The aim of WG 145 is to develop a user-friendly comprehensive chemical speciation model of seawater and related natural waters. PTB has, together with the metrology institutes of the US, France and Japan, carried out new potentiometric measurements, that will be used by WG145 to characterize the thermodynamic properties and speciation in the major and minor components of seawater, and in the aqueous buffers used to calibrate instruments for measuring pH, which includes working on an uncertainty analysis of currently available data and "Pitzer" speciation models.

PTB German National Metrology Institute
Working Group 7.42, Applied Thermometry
Dr. Steffen Rudtsch

Projects:

1. Measurements of the speed of sound in water, heavy water and seawater.

Ruhr University Bochum
Faculty of Mechanical Engineering, Chair of Thermal Turbomachines and Aeroengines
Prof. Dr. Francesca di Mare

Projects:

1. Implementation of the Spline Based Table Lookup Method (SBTL) into the in-house code Shar-C for high-fidelity, scale-resolving calculations of unsteady, turbulent, condensing wet steam flows in low-pressure turbines.
   - The in-house, density-based CFD solver Shar-C is specifically optimized for the computation of thermodynamically complex flows as, e.g., non-equilibrium condensing wet steam (SBTL based), real gas and real gas mixtures (SBTL and Peng-Robinson based) and combustion.
   - At current times, wet steam flows are treated by means of the mono-dispersed Source-Term Euler-Euler model and the non-equilibrium condensation effects are modeled based on the classical theory of droplet nucleation and droplet growth.
   - A considerable computational speed is obtained, where the SBTL method shows an overhead of only 2% compared to a baseline ideal gas computation; a full condensation computation is only connected to an overhead of 26%.
   - For high quality LES computations, the solver is equipped with a hybrid, low-dissipation spatial discretization scheme for accurate treatment of turbulence in presence of shock waves and discontinuities due to condensation.
   - The first large eddy simulation of a realistic condensing wet steam flow was presented in 2020: Overall, the LES results are much better able to reproduce the experimental data compared to standard RANS and URANS computations. Based on the SBTL and a highly-optimized code, the LES on a grid with 48 million cells could be conducted in a computational time of 1000 CPU weeks.
2. Implementation of extensions of the SBTL method to humid air and other flow media like CO2 into the in-house code Shar-C.
3. Implementation of the SBTL method into an in-house high-order finite-difference code targeted towards direct numerical simulations of compressible real gas flows for computations on GPUs.
4. Implementation of a new unstructured FVM and high-order DG solver for the solution of complex thermodynamic flows (like condensing wet steam flows) in complex geometries and for scale-

resolving computations.

5. Investigation the use of Physics Informed Artificial Neural Networks for the Physics Recovery to advance the state of condensation Modeling.

Recent Publications

- Post, P.; Winhart, B.; di Mare, F.:
  Large Eddy Simulation of a Condensing Wet Steam Turbine Cascade.
  J. Eng. Gas Turbines Power, GTP-20-1526.
- Post, P.; Winhart, B.; di Mare, F.:
  Large Eddy Simulation of a Condensing Wet Steam Turbine Cascade.
  ASME Paper GT2020-16064, Proceedings of ASME Turbo Expo 2020: Turbine Technical Conference and Exposition GT2020, London, UK.
- Karaefe, E. K.; Post, P.; Sembritzky, M.; Schramm, A.; Kunick, M.; Gampe, U.; di Mare, F.:
  Numerical Investigation of a Centrifugal Compressor for Supercritical CO2 Cycles.
  ASME Paper GT2020-15194, Proceedings of ASME Turbo Expo 2020: Turbine Technical Conference and Exposition GT2020, London, UK.

Ruhr University Bochum
Faculty of Mechanical Engineering, Department of Thermodynamics
Prof. Dr.-Ing. Roland Span

Projects:

- Our project on hydrate formation, which is carried out in cooperation with colleagues from the Institute of Thermomechanics of the Czech Academy of Sciences in Prague and from TU Dresden, has reached its (preliminary) end. With the defense of the thesis of Dr. Sebastian Hielscher the active work ended. Results were published in Journals [1,2] and on national and international conferences. A follow up proposal has been submitted to the German Science Foundation (DFG), involving Dr. V. Vins as “Mercator Fellow”. A decision regarding the proposal is expected by the end of 2021.
- Our work on consideration of salts in water and in mixtures containing water is progressing. It has been shown that the IAPWS seawater equation can be used in Helmholtz-energy based mixture models. This way mixtures with brines can be described using the framework of equations of state established for natural gases and CO_2-rich mixtures. Results were presented on national and international conferences, were presented to IAPWS TPWS by Benedikt Semrau, and were submitted to an international journal [3]. However, the use of the IAPWS seawater model results in restrictions regarding allowable salt composition, salinity and temperature and pressure range. To come to a more general description of brines, the model is currently extended using a Pitzer approach to describe the electrolytes. First results were presented were presented on national and international conferences, and to IAPWS TPWS. The project received funding by the EU / ERA ACT project ELEGANCY and by the Fraunhofer high performance center DYNAFLEX. Currently funding for continued work is missing.

- In particular for CCS application aqueous mixtures with amines are relevant, be it for capture processes, where high amine concentrations are typical, or for transport, where water and amines are minor components in CO_2-rich mixtures. A physically sound description of these mixtures requires models that are able to represent the behavior of reacting systems. Typically, these models are excess Gibbs-enthalpy models (g^E models), which are able to describe phase equilibria relatively well, but which do not describe properties of homogeneous states and of coexisting phases well. A project carried out in cooperation with a colleague at the NTNU in Trondheim (Prof. Jana Poplsteinova

Jakobsen) aims at the implementation of a g^E model into a Helmholtz mixture model to combine the description of VLE of reacting mixtures with the accuracy of Helmholtz mixture models for the description of thermodynamic properties.

First results are promising and have been presented on national and international conferences by Tobias Neumann; a journal publication is under preparation. The project received funding by the Norwegian CCS Center (NCCS) led by SINTEF Energy. Currently funding for continued work is missing.

[1] *S. Hielscher, V. Vinš, A. Jäger, J. Hrubý, C. Breitkopf, and R. Span:* A new approach to model mixed hydrates. In: Fluid Phase Equilibria 459, 170-185 (2018).
[2] *S. Hielscher, B. Semrau, A. Jäger, V. Vinš, C. Breitkopf, J. Hrubý, and R. Span:* Modification of a model for mixed hydrates to represent double cage occupancy. Fluid Phase Equilibria 490, 48-60 (2019).
[3] *B. Semrau, S. Hielscher, M. Thol, and R. Span:* Combination of Gibbs and Helmholtz energy equations of state in a multiparameter mixture model using the IAPWS seawater model as an example. Submitted to Int. J. Thermophysics (2021).

Technical University of Dresden
Institute of Power Engineering, Chair of Technical Thermodynamics
Prof. Dr. Cornelia Breitkopf, Dr. Andreas Jäger

Projects:

- Development of an algorithm for fitting the model parameters of the combination of the multi-fluid mixture model with the excess Gibbs energy models UNIFAC and COSMO-SAC. In a first step, the algorithm will be applied for fitting water + linear alkane mixtures with the focus on Henry coefficients for these mixtures.

Zittau/Goerlitz University of Applied Sciences
Faculty of Mechanical Engineering Zittau / KCE-ThermoFluidProperties, Dresden
Prof. Dr. Hans-Joachim Kretzschmar, Dr. Sebastian Herrmann

Projects

1. Development of a new ASHRAE standard for calculating thermodynamic properties of moist air, ASHRAE Project SPC-213P, Method for Calculating Moist Air Thermodynamic Properties.
   The vapor pressure and saturation temperature equations of the IAPWS-IF97 Industrial Formulation and the melting pressure equation of the IAPWS Formulation 2011 are being incorporated into the ASHRAE Standard, Method for Calculating Moist Air Thermodynamic Properties.
2. Preparation of Chapter 1 Psychrometrics for the 2021 ASHRAE Handbook of Fundamentals.
   The equations for thermodynamic properties of the IAPWS-IF97 Industrial Formulation and the equations for transport properties of the IAPWS Formulation 2008 for the viscosity and the IAPWS Formulation 2011 for the thermal conductivity of water have been incorporated into the 2021 ASHRAE Handbook of Fundamentals.

Recent Publications

- Herrmann, S.; Kretzschmar, H.-J.; Aute, V. C.; Gatley, D. P.; Vogel, E.:
  Transport Properties of Real Moist Air, Dry Air, Steam, and Water.
  Science and Technology for the Built Environment, 27 (2021), pp. 393 - 401.
  DOI: 10.1080/23744731.2021.1877519.

Zittau/Goerlitz University of Applied Sciences
Faculty of Mechanical Engineering, Dept. of Energy Systems Technology, Zittau
Prof. Dr. Matthias Kunick

Projects

1. Development of fast property-calculation algorithms for water and steam in thermo-hydraulic process simulations
   - Development of the property library libSBTL95 for water and steam considering special requirements of the thermo-hydraulic code ATHLET, developed by the German Society of Global Research for Safety (GRS), Garching. Fluid properties are extrapolable beyond physical boundaries in order to satisfy the demands of the solver algorithm in ATHLET. The library is based on IAPWS-95 and the Spline-Based Table Look-Up Method (SBTL) in order to provide high accuracy and computational efficiency.
   - Implementation and verification of the property library libSBTL95 in ATHLET.
2. Development of fast property-calculation algorithms for gaseous mixtures of water with non-condensable gases in thermo-hydraulic process simulations:
   - Development of computationally efficient algorithms for the properties of gaseous mixtures of water vapor with Ar, CO, CO2, He, H2, N2, and O2. The mixture model combines the ideal mixing of real fluids with a residual part obtained from a virial-mixing approach or a one-fluid model.
   - Implementation and verification of the property library libSBTL95 in ATHLET.
3. Application of the Spline-Based Table Look-Up Method (SBTL) to humid air
   - SBTL functions have been developed for water and steam as well as for dry air and the enhancement factor. These SBTL functions have been implemented into a new property library for humid air which is successfully applied at the Fraunhofer UMSICHT, Oberhausen, for the simulation of Advanced Adiabatic Compressed Air Energy Storages (AA-CAES).

Recent Publications

- Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.;
  Friend, D. G.; Harvey, A. H.:
  Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL).
  J. Eng. Gas Turbines Power, in preparation.

Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, September 17, 2021

Japanese National Committee, Chaired by Professor Kenji Yasuoka
International Association for the Properties of Water and Steam
c/o The Japan Association for the Properties of Water and Steam
Chaired by Professor Kenji Yasuoka
3-14-1 Hiyoshi, Kohoku-ku,
Yokohama 223-8522, Japan

I. Overview:

The Japan National Committee of IAPWS continues to endeavor to make closer and innovative interactions between engineering and academic groups with respect to the international and domestic energy-related issues. The key points of our attention are cleaner, greener, and more sustainable energy as well as high efficiency and safety. We are discussing the science and engineering of fuels, boilers, turbines, and water-treatment. Now we take it into account the power generation from geothermal and biomass energies. Our activities in the publication are shown below.

II. Recent Publications:

Yasuoka, Kenji
Professor, Department of Mechanical Engineering, Keio University
email: yasuoka@mech.keio.ac.jp
URL: https://k-ris.keio.ac.jp/html/100011311_en.html

On effective radii of dodecahedral cages in semiclathrate hydrates for van der Waals and Platteeuw model
Muromachi, S., Takeya, S., Yuhara, D., Yasuoka, K.
Fluid Phase Equil., 527, 112846, 2021

The influence of random number generation in dissipative particle dynamics simulations using a cryptographic hash function
Okada K, Brumby P.E, Yasuoka K.
PLOS ONE, 16, e0250593, 2021

Phase Transitions and Hysteresis for a Simple Model Liquid Crystal by Replica-Exchange Monte Carlo Simulations
Kowaguchi, A., Brumby, P. E., Yasuoka, K.
Molecules, 26, 1421, 2021

A biointerface effect on the self-assembly of ribonucleic acids: A possible mechanism of RNA

polymerisation in the self-replication cycle
Arai, N., Kobayashi, Y., Yasuoka, K.
Nanoscale, 12, 6691, 2020

Mechanism for H_2 diffusion in sII hydrates by molecular dynamics simulations
Hasegawa, T., Brumby, P. E., Yasuoka, K., Sum, A. K.
J. Chem. Phys, 154, 054706 (10 pages), 2020

Dataflow programming for the analysis of molecular dynamics with AViS, an analysis and visualization software application
Pua, K., Yuhara, D., Ayuba, S., Yasuoka, K.
PLOS ONE, 15, e0231714 (13 pages), 2020

The acidic tail of HMGB1 regulates its secondary structure and conformational flexibility: A circular dichroism and molecular dynamics simulation study
Anggayasti, W. L., Ogino, K., Yamamoto, E., Helmerhorst, E., Yasuoka, K., Mancera, R. L.
Comput. Struct. Biotechnol. J., 18, 1160-1172, 2020

Matubayasi, Nobuyuki
Professor, Graduate School of Engineering Science, Osaka University
email: nobuyuki@cheng.es.osaka-u.ac.jp
URL: http://www.cheng.es.osaka-u.ac.jp/matubayasi/english/index.html

Solvation energetics of protein and its aggregates analyzed by all-atom molecular dynamics simulation and the energy-representation theory of solvation
Matubayasi N.
Chem. Comm., 57, published online, 2021 DOI: 10.1039/D1CC03395F

Crystallization of Polyethylene Brushes and Its Effect on Interactions with Water
Yagasaki T., Matubayasi N.
Macromolecules, 54, published online, 2021 DOI: 10.1021/acs.macromol.1c01145

Temperature Dependence of Sorption
Shimizu S., Matubayasi N.
Langmuir, 37, published online, 2021 DOI: 10.1021/acs.langmuir.1c01576

Breakdown of the Stokes-Einstein relation in supercooled liquids: a cage-jump perspective
Pastore R., Kikutsuji T., Rusciano F., Matubayasi N., Kim K., Greco F.
J. Chem. Phys., 155, published online, 2021 DOI: 10.1063/5.0059622

Cooperative Sorption on Porous Materials
Shimizu S., Matubayasi N.
Langmuir, 37, 10279-10290, 2021

Water Dissolved in a Variety of Polymers Studied by Molecular Dynamics Simulation and a Theory of Solutions
Kojima H., Handa K., Yamada K., Matubayasi N.
J. Phys. Chem. B, 125, 9357-9371, 2021

Molecular insights on confined water in the nanochannels of self-assembled ionic liquid crystal Ishii Y., Matubayasi N., Watanabe G., Kato T., Washizu H.
Sci. Adv., 7, eabf0669, 2021

Construction of isostructural hydrogen-bonded organic frameworks: limitations and possibilities of pore expansion
Suzuki Y., Gutiérrez M., Tanaka S., Gomez E., Tohnai N., Yasuda N., Matubayasi N., Douhal A., Hisaki I.
Chem. Sci., 12, 9607-9618, 2021

Adsorbate-adsorbate interactions on microporous materials
Shimizu S., Matubayasi N.
Micropor. Mesopor. Mater., 323, 111254 (8 pages), 2021

Sorption: A Statistical Thermodynamic Fluctuation Theory
Shimizu S., Matubayasi N.
Langmuir, 37, 7380-7391, 2021

Transition pathway of hydrogen bond switching in supercooled water analyzed by the Markov state model
Kikutsuji T., Kim K., Matubayasi N.
J. Chem. Phys., 154, 234501 (7 pages), 2021

Understanding the scaling of boson peak through insensitivity of elastic heterogeneity to bending rigidity in polymer glasses
Tomoshige N., Goto S., Mizuno H., Mori T., Kim K., Matubayasi N.
J. Phys.: Condens. Matter, 33, 274002 (7 pages), 2021

Cooperativity in micellar solubilization
Shimizu S., Matubayasi N.
Phys. Chem. Chem. Phys., 23, 8705-8716, 2021

Spatial-Decomposition Analysis of Electrical Conductivity in Mixtures of Ionic Liquid and Sodium Salt for Sodium-Ion Battery Electrolytes
Hakim L., Ishii Y., Matubayasi N.
J. Phys. Chem. B, 125, 3374-3385, 2021

Implicit function theorem and Jacobians in solvation and adsorption
Shimizu S., Matubayasi N.

Physica A, 570, 125801 (11 pages), 2021

Phase stability condition and liquid-liquid phase separation under mesoscale confinement
Shimizu S., Matubayasi N.
Physica A, 563, 125385 (13 pages), 2021

Fluctuation adsorption theory: quantifying adsorbate-adsorbate interaction and interfacial phase transition from an isotherm
Shimizu S., Matubayasi N.
Phys. Chem. Chem. Phys., 22, 28304-28316, 2020

Solubilization Power of Surfactant-Free Microemulsions
Schöttl S., Matubayasi N., Horinek D.
Phys. Chem. Chem. Phys., 22, 22185-22189, 2020

Intensive nature of fluctuations: Reconceptualizing Kirkwood-Buff theory via elementary algebra
Shimizu S., Matubayasi N.
J. Mol. Liq., 318, 114225 (8 pages), 2020

Transport Properties of Ionic Liquid and Sodium Salt Mixtures for Sodium-Ion Battery Electrolytes from Molecular Dynamics Simulation with a Self-Consistent Atomic Charge Determination
Hakim L., Ishii Y., Matsumoto K., Hagiwara R., Ohara K., Umebayashi Y., Matubayasi N.
J. Phys. Chem. B, 124, 7291-7305, 2020

Learning reaction coordinates via cross-entropy minimization: Application to alanine dipeptide Mori Y., Okazaki K., Mori T., Kim K., Matubayasi N.
J. Chem. Phys., 153, 054115 (8 pages), 2020

Cavity Particle in Aqueous Solution with a Hydrophobic Solute: Structure, Energetics, and Functionals
Zhang B.W., Matubayasi N., Levy R.M.
J. Phys. Chem. B, 124, 5220-5237, 2020

Thermodynamic stability condition can judge whether a nanoparticle dispersion can be considered a solution in a single phase
Shimizu S., Matubayasi N.
J. Colloid Interface Sci., 575, 472-479, 2020

Chain-Increment Method for Free-Energy Computation of a Polymer with All-Atom Molecular Simulations
Yamada K., Matubayasi N.
Macromolecules, 53, 775-788, 2020

Self-Consistent Scheme Combining MD and Order N DFT Methods: An Improved Set of Nonpolarizable Force Fields for Ionic Liquids
Ishii Y., Matubayasi N.

J. Chem. Theory Comput., 16, 651-665, 2020

Solvation Thermodynamics from the Perspective of Endpoints DFT,
Levy R.M., Matubayasi N., Zhang B.W.
J. Phys. Chem. B, 124, 11771-11782, 2020

Yohei, Kayukawa
Senior Researcher, Mass Standards Group, Research Institute of Engineering Measurement
National Metrology Institute of JAPAN (NMIJ), National Institute of Advanced Industrial Science and Technology (AIST)
Email: kayukawa-y@aist.go.jp

Evaluation of estimation accuracy of saturated properties and theoretical performance for refrigerants with ECS model
Teraishi, R., Kayukawa, Y., Akasaka, R., Jeong, J., Saito, K.
Trans. Jpn. Soc. Refrig. Air Cond. Eng., 38, 3, 2021, in press (in Japanese).

Universal Parameters of the Extended Corresponding States (ECS) Model for Hydrofluoroolefin Refrigerants
Teraishi, R., Kayukawa, Y., Akasaka, R., Saito, K
Int. J. Refrig., 2021, in press. DOI: 10.1016/j.ijrefrig.2021.08.013

pρT property measurements for HFO-1123 by a single sinker magnetic levitation densimeter.
Kayukawa, Y.
Int. J. Refrig., 119, 349–355, 2020

Dipole moment and heat capacity in the ideal gas state derived from relative permittivity and speed of sound measurements for HFO-1123 and HCFO-1224yd(Z).
Kano, Y., Kayukawa, Y., Fujita, Y.
Int. J. Refrig., 118, 354–364, 2020

Yoshida, Ken
Associate Professor, Department of Applied Chemistry, Graduate School of Technology, Industrial and Social Sciences, Tokushima University
email: yoshida.ken@tokushima-u.ac.jp
URL: http://pub2.db.tokushima-u.ac.jp/ERD/person/189117/work-en.html

Solvation shell dynamics of supercritical water-cyclohexane mixtures in relation to the translational and rotational dynamics as studied by molecular dynamics simulation
Yoshida K., Yoshioka H.
AIP Advances, 11, 075219, 2021

Temperature Dependence of Water on Functionalized Graphite

Horikawa T., Yuasa R., Yoshida K., Do D.D.
Carbon, 183, 380-389, 2021

^{14}N NMR Evidence for Initial Production of NH_3 Accompanied by Alcohol from the Hydrolysis of Ethylamine and Butylamine in Supercritical Water
Yoshida K., Yoshioka H., Ushigusa N., Nakahara M.
Chem. Lett, 50, 316-319, 2021

Nakahara, Masaru
Professor Emeritus, Institute for Chemical Research, Kyoto University
Email: nakahara@scl.kyoto-u.ac.jp

^{14}N NMR Evidence for Initial Production of NH_3 Accompanied by Alcohol from the Hydrolysis of Ethylamine and Butylamine in Supercritical Water
Yoshida K., Yoshioka H., Ushigusa N., Nakahara M.
Chem. Lett 50, 316-319, 2021

Dynamics and Chemical Reactions of Supercritical Water
Nakahara M.
Last Activity Report of the 183rd JSPS Committee on Advanced Water Science and Engineering, 18-19, 2021 (in Japanese)

Miyamoto, Hiroyuki
Associate Professor, Department of Mechanical Systems Engineering, Toyama Prefectural University
email: miyamoto@pu-toyama.ac.jp

Measurement of the vapour–liquid equilibrium properties of binary mixtures of the low-GWP refrigerants R1123 and R1234yf
Miyamoto H., Nishida M., Saito T.
J. Chem. Thermodyn., 158, 106456, 2021

Vapor–Liquid Equilibrium Property Measurements for R32/R1234yf Binary Mixtures in Low R32 Concentration
Yamada T., Miyamoto H., Sakoda N., Higashi Y.
Int. J. Thermophys., 41, 167, 2020

Measurement of the vapor–liquid equilibrium properties of the binary low GWP refrigerant R32/R1123
Miyamoto H., Saito T., Sakoda N., Perera U., Ishii T., Thu K., Higashi Y.
Int. J. Refrig., 119, 340-348, 2020

Sawatsubashi, Tetsuya
Team Manager, Research & Innovation Center, Mitsubishi Heavy Industries, Ltd.
Email: tetsuya.sawatsubashi.np@mhi.com

Study of A Sampling Method by Wiping for Analysis of Deposit on a Steel Surface
Katada, M., Noda, S., Yoshida, M., Ureshino, A., Ohtsuka, M., Sawatsubashi, T.
Therm. Nucl. Power, in press.

Current Status and New Technology of Water Treatment in Thermal Power Plants (Non-Toxic Oxygen Scavenger, Japanese Industrial Standard Revision, Water Quality Diagnostic
Akamine, H., Nakamoto, M., Sawatsubashi, T., Nakatsuchi, Y., Tamura, K.
The Piping Engineering, 853, 63, 70-74, 2021 (in Japanese)

The Swiss National Committee

International Association for the Properties of Water and Steam

Report on IAPWS related activities – September 2020 / September 2021

Submitted to the EC Meeting of IAPWS – September 2021

National Committee Contacts:

President: Vacant

Secretary: Tapio Werder, E-mail: tapio.werder@ppchem.com

Following Individuals participated in the research into the thermophysical properties and chemical processes:

- Dr. Robert Svoboda, Svoboda Consulting, Wettingen,
  E-Mail: r.l.svoboda@swissonline.ch
- Michael Rziha, PPCHEM AG Hinwil, E-Mail: michael.rziha@ppchem.com
- Marco Lendi, Swan Analytical Instruments, Hinwil, E-Mail: marco.lendi@swan.ch
- Tapio Werder, PPCHEM AG, Hinwil, E-Mail: tapio.werder@ppchem.com

Research activities in the reporting period:

No new projects were reported

Contributions to current IAPWS activities:

Chairman PCC Working Group: Michael Rziha

Chairman of PCC Sub-Task Group: Technical Guidance Document Chemistry Management in Generator Water Cooling during Operation and Shutdown: Robert Svoboda

Status of Associate Membership to IAPWS:

Up to now, no team of sponsors to commit on mid- or long-term to a regular Swiss membership fee has yet been assembled. Activities were therefore limited to few individuals. Due to COVID-19, no activities as planned were possible. The board of SCPWS is currently planning for 2022 to find new participating institutions in Switzerland. Marco Lendi resigned from Presidency at the end of 2020. New President to be announced in 2022.

- It is therefore requested to extend the Associate Membership for another term.

Tapio Werder, September 2021

U.S. National Committee to IAPWS
2021 Report on Activities of Potential Interest to IAPWS

7 September 2021

Communicated from the Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO:

In an IAPWS project, in collaboration with Marc Assael (Aristotle University, Greece) and Jan Sengers (University of Maryland and NIST), new viscosity and thermal conductivity correlations for heavy water have been developed. The viscosity formulation has been approved as an IAPWS Release (IAPWS R17-20) and was published: M.J. Assael, S.A. Monogenidou, M.L. Huber, R.A. Perkins, and J.V. Sengers, "New International Formulation for the Viscosity of Heavy Water," *Journal of Physical and Chemical Reference Data* **50**, 033102 (2021). This article was selected by the American Institute of Physics as a Scilight feature (09 July 2021). The thermal conductivity formulation (which makes use of the viscosity formulation) is being evaluated for adoption as an IAPWS Release, and a paper is in preparation to be submitted to the *Journal of Physical and Chemical Reference Data*.

A collaboration has begun between NIST and the group of Prof. Tremaine at the University of Guelph with the objective of developing a standard formulation for the static dielectric constant of heavy water. Thus far, we have gathered the available experimental data and made preliminary comparisons based on the existing H_2O correlation in order to see where there are gaps in the data that might need to be filled in based on H_2O behavior. It is hoped that a new formulation will be ready before the 2022 IAPWS meeting.

Communicated from OLI Systems, Cedar Knolls, NJ

Aqueous chemistry of rare earth elements

OLI Systems has continued its participation in the activities of DOE's Critical Materials Institute (CMI). Under the auspices of CMI, recent work was focused on (1) development of simulation methodology to optimize the recovery of rare earths from end-of-life electronics, (2) simulation of recovery of metals from lithium-ion battery cathodes using biological media, and (3) development of a thermodynamic model for rare earth fluorides in aqueous environments. The results of the work on project (1) have been published in the following paper:

- T.E. Lister, M. Meagher, M.L. Strauss, L.A. Diaz, H.W. Rollins, G. Das, M.M. Lencka, A. Anderko, R.E. Riman, and A. Navrotsky, *Recovery of Rare Earth Elements from Recycled Hard Disk Drive Mixed Steel and Magnet Scrap*, chapter 15 in Rare Metal Technology 2021, edited by G. Azimi, T. Oishi, K.M.M. Forsberg, H. Kim, S. Alam, A.A. Baba, and N.R. Neelameggham, The Minerals, Metals & Materials Series, Springer (2021), pp. 139-154.

Aqueous chemistry for carbon capture and transportation

In collaboration with the Institute for Energy Technology (Norway), OLI has continued its work on developing simulation capabilities to predict the risk of corrosion in CO_2 transportation. Recent work was focused on the effects of organic impurities including monoethylene glycol, methanol, and acetaldehyde.

Aqueous chemistry of boric acid and borates up to high temperatures
Speciation and solubility of boric acid and various borates (primarily lithium, sodium, potassium, calcium, magnesium and zinc borates) at high temperatures is important for nuclear power generation. Recently, a comprehensive experimental study of borate speciation has been conducted using electrical conductivity measurements and Raman spectroscopy and published in a series of papers by Tremaine and coworkers. This experimental database has formed the foundation for revising OLI's Mixed-Solvent Electrolyte (MSE) model for borate systems. Work has been completed on borate thermodynamics in the absence of other anions. Currently, work is in progress on incorporating the effects of chlorides and sulfates.

Communicated From University of Washington, Department of Earth and Space Sciences Seattle, WA

The University of Washington team (J.M. Brown, E. Abramson, B. Journaux) continue to improve computer access to thermodynamic properties of fluids and ices and have investigated thermodynamic properties of ammonia-water solutions. Manuscripts in preparation contain a full accounting of the work. Here, a brief summary is provided.

• Thermodynamic properties of the ices (Journaux et al 2020) and various solutions are contained in the SeaFreeze database. Open-source software (including matlab and python code and a GUI-based application that run in both Windows and MacOS: https://github.com/Bjournaux/SeaFreeze/tree/master/SeaFreezeGUI) is available through seafreeze.org. The SeaFreeze GUI application, requiring no user coding, generates figures and output tables of user-specified properties for water and all ice polymorphs between 180 K and 500 K to 2300 MPa.

• Speeds of sound in solutions with concentrations ranging from pure water to x=0.3 (mole fraction ammonia) taken in our laboratory, to pressures of 700 MPa over a range of temperatures, provide the high-pressure constraints for a new Gibbs energy representation.

• Our analysis, further discussed below, requires accurate fluid densities, specific heats and enthalpies at a single, (low) pressure.

• The resulting equation of state was tested against the 1 bar melting point depression and new high-pressure melting point determinations of ices (ice Ih and ice VI) measured in our laboratory for several concentrations of ammonia-water solutions.

The IAPWS formulation for the ammonia-water equation of state (Tillner-Roth and Friend, 1998), or TRF hereafter, is based primarily on measurements at pressures below 20 MPa, and one study to 40 MPa (Harms-Watzenberg, 1995). Although measurements from different studies disagree by far more than their precision, or even stated uncertainties, there are consistent, systematic deviations evident between the bulk of the literature data and the current IAPWS Guideline. For instance,

- density: 0.4 % deviations around room temperature

- specific heat: 2 % at room temperature and x<0.3, rising to 10 % at 250 K and x>0.3
- enthalpy: deviations of 200 J/mol
- pressures at vapor-liquid equilibrium (*VLE*): 10 % systematic deviation at 20 °C
- speeds of sound: 3 % deviation at the largest concentration (x=0.15) previously measured (Marks, 1960).

This suggests that the equation of state, currently expressed in terms of a library of common functions (e.g., polynomials, exponentials) might more accurately be expressed in terms of more flexible local basis functions in the form of tensor b-splines (Brown 2018). To this purpose, data for *Cp* (x,T) and r(x,T), gathered from the literature, were expressed as fractional differences from the TRF equation of state and surfaces in concentration and temperature loosely fit to these deviations.

New high-pressure and below room temperature melting points extending to 220 K and up to 1700 MPa were measured in a cryogenically cooled diamond anvil cell. Pressures were measured using the fluorescence of ruby (Journaux et al. 2020). The liquidus was determined when the volume of the ice crystal was visually smaller than 0.5% of the pressure chamber, following the procedure in Journaux et al. (2013). The new melting point determinations in aqueous solutions with ammonia align well with predictions based on the new ammonia-water Gibbs energy representation and the ices (Journaux et al 2020). Thus, the stabilities of high-pressure ice phases are reliably predicted at all pressure covered by the new representation.

Group Publications Cited:

Brown, J.M., (2018) *Local basis function representations of thermodynamic surfaces: Water at high pressure and temperature as an example*, Fluid Phase Equilibria, 463C, 18-31
doi:10.1016/j.fluid.2018.02.001

Bollengier, O., Brown, J.M., Shaw, G.H., (2019) *Thermodynamics of pure liquid water: Sound speed measurements to 700 MPa down to the freezing point, and an equation of state to 2300 MPa from 240 to 500 K*, J. Chem. Phys. 151, 054501
Doi 10.1063/1.5097179

Journaux, B., J.M. Brown, A. Pakhomova, I. Collings, S. Petitgirard, P. Espinoza, J. Ott, F. Cova, G. Garbarino, M. Hanfland (2020) *Gibbs energy of ices III, V and VI: Wholistic thermodynamics and elasticity of the water phase diagram to 2300 MPa,*
J. Geophys. Res. Planets, 125, doi: e2019JE006176

Miscellaneous Items

The History and Heritage Committee of ASME (American Society of Mechanical Engineers) is designating “Standardized Steam Property Tables” as a Historic Mechanical Engineering Landmark. This designation is given to a few artifacts and achievements each year; the designation in 2021 reflects the centennial of the ASME’s efforts on standardized steam tables, which began in 1921. The

accompanying brochure and (virtual) plaque have been drafted, and the official landmark designation will be made on the ASME website in Fall 2021.

The 21st Symposium on Thermophysical Properties was held as a virtual event from June 20 to 25, 2021, as part of the triennial series of conferences organized by the Joint ASME-AIChE Committee on Thermophysical Properties. Of interest to IAPWS, there were four sessions devoted to the Properties of Aqueous Systems comprising 17 talks; more than 30 additional talks involving water or aqueous systems were presented under other topic areas (e.g., molecular simulation or experimental methods). Properties of hydrate systems represented another significant area of interest within the Symposium. The website at https://thermosymposium.org provides a complete set of abstracts, including of those talks indicated above.