#### 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

#### **EXECUTIVE SECRETARY**

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#### **Minutes of the Virtual Meeting**

of the

#### **Executive Committee**

of the

#### International Association for the Properties of

Water and Steam

11th September 2020

#### **Prepared by Barry Dooley**



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## **IAPWS Minutes**

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#### Minutes of the Virtual Meeting

#### of the Executive Committee of the International Association for the Properties of Water and Steam

#### 11<sup>th</sup> September 2020

At 12:00 noon in the UK, the President of IAPWS, Dr. Jan Hruby welcomed the Executive Committee (EC) and other IAPWS members to the Virtual Executive Committee (EC) Meeting operating on ZOOM Cloud. All of the Member and Associate Member countries of IAPWS were in attendance with the exception of Argentina/Brazil, France and Greece. In total there were 25 people assembled for the EC meeting.

#### 1. <u>Adoption of Agenda</u>

Provisional agendas had been e-mailed to all IAPWS members by the Executive Secretary in July 2019. There were no additions and the final agenda forms Attachment 1 of these minutes.

#### 2. IAPWS Business and Appointment of Committees

2.1 <u>IAPWS Business Since Last EC Meeting in Banff, Canada on 4<sup>th</sup> October 2019 (Note: this is an informational item added to the minutes following the EC meeting)</u>

The following documents were circulated to the National Committees during the year since the Banff meeting for postal ballot:

- *ICRN 31 on New Thermodynamic Data for Ordinary Water.* Banff EC Minute 7.1 indicated that the TPWS WG voted to approve the ICRN, subject to some editorial corrections and addition of an item on surface tension. The EC had approved the WG request to authorize a Postal Ballot for the ICRN, to be conducted after these small edits. The document was circulated for a Postal Ballot on 11<sup>th</sup> October 2019. No objections were received by 11<sup>th</sup> February 2020, so the ICRN became an official IAPWS document (ICRN-31).
- *Guideline for Surface Tension of Seawater*. Banff EC Minute 9.2 indicated that an Evaluation Task Group had reviewed the document and that the EC had approved the joint WG (TPWS and SCSW) request to authorize a Postal Ballot once editorial changes had been completed. The document was circulated for a Postal Ballot on 19<sup>th</sup> December 2019. No objections were received by 19<sup>th</sup> March 2020, so the Guideline became an official IAPWS document (IAPWS G14-19).

#### 2.2 IAPWS Awards Committees

#### 2.2.1 Honorary Fellow Award Committee

A committee of Nakahara (Chairman) and Harvey were selected for the 2020 award but no nomination was made. It was suggested that the same committee remain in place for 2021 with the Executive Secretary as ex. Officio member.

#### Action: Nominations are due to the Executive Secretary by 31<sup>st</sup> January 2021.

#### 2.2.2 <u>Helmholtz Award Committee</u>

The 2020 Helmholtz Award committee (Chair: Nemec) reviewed the 2020 proposals and had agreed on a nomination. Unfortunately, the Torino 2020 meeting was cancelled, and the committee suggested that the Awardee (Dr. Ishiyama, Toyama University, Japan) be asked to present a Helmholtz Award lecture at the Torino 2021 meeting. A Helmholtz Award committee would be selected for 2021.

The Executive Secretary reminded the EC that the Helmholtz Committee for the 2021 award would consist of a member from Japan (Chair) (Yasouka), New Zealand (Addison), SIAPWS, Russia and USA (Anderko). Each National Committee provided the names indicated.

#### Action: Nominations are due to the Executive Secretary by 31<sup>st</sup> January 2021.

#### 2.3 Host Country for 18<sup>th</sup> ICPWS

Banff 2019 EC Minutes 2.5 and 17.3 discussed the 18<sup>th</sup> ICPWS and the EC had requested the Head of the US National Committee (Friend) to report back at the 2020 EC meeting with details on hosting the 18<sup>th</sup> ICPWS. Friend indicated the following points:

- The U.S. National Committee will host the 18<sup>th</sup> ICPWS in conjunction with the ASME Energy Storage and Conversion Segment that will provide logistical support
- Organization will involve a Local Organizing Committee (LOC) and an International Program Committee IPC (including IAPWS Officers and WG Chairs)
- The initial thoughts and plan for the conference are that it will follow the traditional ICPWS format and be held in early to mid-September (TBD) in the Denver, Colorado Area of the USA at a hotel to be decided
- Because of the uncertainty, the US National Committee has discussed some contingency planning which has included: travel restrictions, restrictions on gatherings, consideration of some virtual content, planning for smaller attendance and a shorter conference with more WG sessions during the week.

#### 2.4 <u>Statutes and By-Laws</u>

To ensure appropriate and non-commercial use of the IAPWS name and logo, a small Statutes and By-Laws committee was formed with Harvey as Chair and Addison as member with the President and Executive Secretary as ex-officio. Harvey provided information on a draft for a suggested new By-Law 10. This 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. It was also suggested that the IAPWS name and/or logo should not be used in a manner that gives the appearance of promoting a commercial process or entity.

This raised a number of points of discussion by the EC on defining the aspects of commercialization and on documenting the use of an IAPWS formulation or Technical Guidance Document in software or in a scientific paper, as long as such use does not give the appearance of an IAPWS commercial endorsement. Each IAPWS document already includes a statement that publication in whole or in part is allowed in all countries provided that attribution is given to IAPWS. This discussion eventually lead to a proposal that the committee would revise the suggested By-Law 10 and the Executive Secretary would circulate to IAPWS Member Countries for a Postal Ballot.

#### The EC approved this proposal unanimously.

#### 3. Working Groups and Sub-Committee Reports

(Note: The WG Chairs had been asked previous to the EC meeting to only raise items that needed approval by the EC. Also, any WG Minutes are included as attachments to these minutes).

#### 3.1 Thermophysical Properties of Water and Steam (TPWS) Working Group

TPWS Chairman Meier discussed the following items:

3.1.1 Revised Guideline on the Use of Fundamental Physical Constants and Basic Constants of Water.

The TPWS Chair informed the EC that a revision to update the reference to 2018 CODATA to correspond to new section about polarizability of the water molecule. The TPWS WG had approved the revision and the document will become an official IAPWS document on the website.

3.1.2 An evaluation Task Group was appointed in 2019 (Meier (chair), Blahut and Kretzschmar) for Heavy Water Transport Properties. The TPWS Chair made two proposals:

The evaluation of the Release for Viscosity of Heavy Water was finished, but feedback on the evaluation report has not yet been completely received. The TPWS Chair requested the EC to authorize a Postal Ballot for the Release following final feedback and editorial committee review.

#### The EC approved this proposal unanimously.

The Heavy Water Thermal Conductivity draft release has been received by the Task Group and an evaluation will be conducted. The TPWS Chair informed the EC that the Release will be finalized and reviewed by the Editorial Committee. It will then be sent for Postal Ballot in advance of the 2021 meeting.

#### 3.2 Industrial Requirements and Solutions (IRS) Working Group

Minutes of the IRS WG conducted before the EC meeting are in Attachment 2. IRS Chairman Okita requested EC approval for one new IRS WG member who had been approved by the WG:

• Alberto Giuliano Albo (INRIM, Italy).

#### The EC approved this Membership Addition Unanimously.

3.3 <u>Physical Chemistry of Aqueous Systems Working Group (PCAS)</u>

Minutes of the PCAS WG conducted before the EC meeting are in Attachment 3.

#### 4. Editorial Committee Report

Editorial Committee Chairman Harvey reported that in the preceding year, the Editorial Committee (Harvey, Cook and Cooper) had reviewed the *Guideline for Surface Tension of Seawater* mentioned in Minute 2.1.

#### 5. <u>Membership and Associates</u>

#### 5.1 Application of Israel for IAPWS Associate Membership

The Executive Secretary reminded the EC that the application documents for Israel to become an Associate Member had been forwarded to the Heads of IAPWS Member National Committees on 7<sup>th</sup> September 2020. This included a set of ISRAPWS Statutes, and an IAPWS Membership Application Form.

The Chair of ISRAPWS, Yitzhak Nussbaum, was asked to present the application to the EC. Nussbaum is the Chief Chemist in an O&M company that operates four power plants in Israel. The Israeli community of power plants technicians, engineers and chemist is not large, but they started activities about three years ago and have organized two symposia in 2018 and 2019 on power plant operations topics, water treatment, corrosion and related issues. They have formed a National Committee which has a treasurer and secretary.

Nussbaum then on behalf of the Israeli steam and water industries and community requested EC that ISRAPWS become an Associate Member of IAPWS.

#### The EC approved ISRAPWS as an Associate Member of IAPWS Unanimously.

#### 5.2 <u>Reports on Current Associate Members</u>

<u>Status Report on IAPWS Associate Member, Egypt.</u> The Head of the Egypt National Committee, Khalifa, reported that unfortunately because of personal and business reasons there has not been any IAPWS activities during 2020. The National Committee intends to reactivate before the 2021 IAPWS meetings in Torino and will report then.

<u>Status Report on IAPWS Associate Member, Greece.</u> The Head of the Greece National Committee (HIAPWS), Kastanaki, could not attend the EC meeting. The Executive Secretary reported that the HIAPWS had held a steam/water symposium in 2019 with representatives of the power industry.

<u>Status Report on IAPWS Associate Member, India.</u> The Head of the India National Committee (INDIAPWS), Bhattacharyya, reported that during the first year of IAPWS membership, there had been a number of activities including a core committee meeting, a half day symposium and a webinar for Indian power companies. The National Committee is in the process of setting up the financial aspects.

<u>Status Report on IAPWS Associate Member, Switzerland.</u> The Head of the Swiss National Committee, Lendi, indicated that activities have been limited. He indicated that Switzerland was willing to host a future annual IAPWS meeting. He also indicated that he would be stepping down and that he would provide information to the Executive Secretary on the new head of the Swiss national committee by the end of 2020.

#### 6. Executive Secretary's Report

#### 6.1 IAPWS Bank Accounts, Financial, Auditors and IAPWS Dues

The Executive Secretary first indicated that all IAPWS Members had paid the 2020 IAPWS dues with the exception of Russia. The head of the Russian National Committee, Orlov, indicated that the payment was in process.

The Executive Secretary then reported that IAPWS is on a sound financial footing with currently about  $\pounds74,00.00$ GBP in total in the UK and US bank accounts. The status as at  $31^{st}$  August 2020 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 2019 financial statements had been forwarded to the IAPWS Auditors in January 2020. Professor Savarik in Czech Republic and Dr. Delfs 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.

Following an indication from the Czech Republic and German Delegate are willing to continue the auditing activity, the Executive Secretary proposed that these organizations be re-appointed to act as auditors.

#### The EC Approved this Unanimously.

The Executive Secretary proposed to the EC that the dues structure for member countries remains unchanged for 2021.

#### The EC Unanimously Agreed to this Proposal.

#### 6.2 <u>Time and Place of the 2021 and 2022 Meetings</u>

<u>2021 IAPWS Meetings.</u> The Italian National Committee were thanked for being flexible over the cancellation of the 2020 IAPWS meetings and for agreeing to host the 2021 meetings. The Head of the Italian National Committee, Lago, provided information on the 2021 IAPWS meetings which will be in Torino, Italy from  $12^{th} - 17^{th}$  September 2021 at the Starhotel Majestic. There is a website for the meeting: <u>http://iapws2021.inrim.it/</u> and registration will open in February 2021.

<u>2022 IAPWS Meetings</u>. The Head of the New Zealand National Committee, Addison, indicated that they were ready and waiting to hold the 2022 IAPWS meetings in New Zealand. The specific dates and location details have not yet been worked out. The EC will be informed at the 2021 meetings in Torino.

#### 7. Election of IAPWS Officers for 2021 and 2022

The Executive Secretary indicated that according to IAPWS By-Law 8, the election of the next Vice President should be made at the end of the EC meeting in even years. The Executive Secretary had checked the recent history and suggest that the US National Committee should be asked to nominate one of their committee members for the position. He then requested the EC to approve this selection.

#### The EC Unanimously Approved this Selection Process.

Action: The US National Committee should inform the Executive Secretary of their agreement to provide, and the choice of a nomination for Vice President after the next meeting of their committee, and before the end of December 2020.

#### 8. <u>Other Business</u>

#### 8.1 <u>Reports from National Committees</u>.

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

Attachment 4
Attachment 5
Attachment 6
Attachment 7
Attachment 8
Attachment 9
Attachment 10
Attachment 11

#### 8.2 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.

#### 9. <u>Closing Remarks and Adjournment</u>

No further business was raised by the EC. The President thanked everybody for participating at this EC meeting. He was thanked for conducting the activities of IAPWS President in 2019 and 2020 and during the serious corona virus pandemic in 2020. The 2020 EC meeting was closed at 1:15 pm in the UK.

#### Agenda. Virtual Meeting of EXECUTIVE COMMITTEE of IAPWS 11<sup>th</sup> September 2020

(12:00 noon in the UK; 13:00 in Europe; 14:00 in Russia; 20:00 in Japan; 8:00 in Canada (New Brunswick); 5:00 in USA (Colorado); 21:00 in Australia; and 23:00 in New Zealand)

- 1. Opening Remarks. IAPWS President Hruby
- 2. IAPWS Business and Appointment of Committees for 2021 Business

2.1 IAPWS Awards for 2021
 <u>Honorary Fellow</u>: Nakahara and Harvey (were assigned for 2020 but no nominations)
 <u>Helmholtz</u>: Japan (Yasouka Chair), New Zealand (Addison), SIAPWS (Jensen), Russia and USA (Anderko). (Note that there was a Helmholtz awardee selected for 2020. Committee decided that a new nomination would also be made for 2021 and both would present in Torino 2021)

- 2.2 Host Country for 18<sup>th</sup> ICPWS. US Chair Friend
- 2.3 Statutes and By-Laws. New By-Law. Committee (Harvey (Chair) and Addison)
- 3. Working Groups and Sub Committee Reports
  - TPWS has one Guideline and one Release for discussion
  - IRS has one membership item for EC approval
  - WG Minutes (if any) will be included in the IAPWS Minutes
- 4. Editorial Committee Report. Chair Harvey.
- 5. Membership and Associates
  - 5.1 Application of Israel for Associate Member. (Nussbaum Chair ISRAPWS)
  - 5.2 Update Reports of Current Associate Members. (The Chairs of Associate Members Egypt, Greece, India and Switzerland)
- 6. Executive Secretary's Report
  - 6.1 IAPWS Bank Accounts, Financials, Auditors and Dues. (Financial Reports sent to EC)
  - 6.2 Time and Place of 2021 (Italy) and 2022 (New Zealand) Meetings.
- 7. IAPWS Officers for 2021/2022.
- 8. IAPWS Country Reports of Activities.
  - National Committee reports will be included in the IAPWS Minutes.
- 9. Other Business



Barry Dooley 6<sup>th</sup> September 2020

## Minutes of the IAPWS working group IRS, On-line meeting, 26. August 2020

(Numbering of the topics follows IRS agenda)

1. The Chair, Nobuo Okita, opened the on-line (Webex) IRS joint meeting at 9:05 (UTC 7:05) am, 26. August 2020. Agenda was adopted without changes only the point 3) Introduction of new member was moved to point 6) Membership.

- 2. Appointed Adam Nový as a clerk of minutes
- 3. Moved to point 6. Membership
- 4. Status of each task of Industrial Requirements and Solutions
  - **4.1 Report of the Task Group "Categories of industrial requirements"** (*N. Okita*, chairs of other WG) N. Okita reported the current status of the TG and summarized the purpose, WG history and schedule of the task. It was presented the structured and extended list of the possible interests as there were about 10 new items added. There are also already inputs by TPWS/SCSW, PCAS and PCC incorporated. From the items list there were 3 topics identified having the main priority for IRS. The "wet steam", "geothermal steam" and its properties & quality and the acid dew point, where it was stated that the ASPEN model is not giving good results. The output from IAPWS is considered to be in form of ICRN or supporting documents like TGD, Guideline and/or Advisory note.

#### TODO:

Keep updating and sharing the categories to all IAPWS members using OPAL and continue evaluating the distance to the IAPWS business.

#### <u>4.2 Report of the Task Group "Wet steam properties Calculation" (A. Nový, J. Hrubý, K. Orlov,</u> <u>R. Span, K. Meier)</u>

A. Nový reported no progress due still missing important input data from experimental research being idle because of power plant business not doing well. Suggested possible directions for future of this TG for discussion.

The following discussion:

F. di Mare mentioned the topic being highly research important and attractive. S. Senoo confirmed similar problems with business idling and lack of data but the high importance of the topic. All members agreed to continue this TG and F. di Mare, S. Senoo and M. Kunick volunteered to join the TG. **TODO**:

Continue keeping the TG alive with shared chairing (e-mail conference), continue the review of literature and test the calculation models on available measured data. Share available experimental data. Try to find joint funding program to support further measurements and wet steam models.

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

S. Senoo presented the request for literature survey regarding coarse water droplets causing erosion. It was explained the purpose and plan for "closing the gap between the knowledge and the TG goal. This suggestion resulted from previous discussion within the other IAPWS WGs. The main areas of interest are 1) measurements data in steam turbines, 2) technologies of measurement instrumentation for visualization and droplet size distributions, 3) atomization models.

The following discussion:

There was discussed the schedule for the suggested literature survey and F. di Mare suggested possibility of contacting scientists related to measurements namely prof. Joos.

**TODO**: Gather and share relevant papers with S. Senoo until March 2021. The papers will then be "processed" by the TG and the summary should be presented and discussed at 2021 meeting.

Regarding measurements and experimental data contact prof. Franz Joos (retired) and/or his successor Dr. Markus Schatz.

#### 4.4 Report of the joint Task Group on ICRN for acid gas dew points (N. Okita, S. Senoo, T. Němec)

N. Okita just summarized the current status as there were no major changes since the last meeting but addition of items on the Categories list in 4.1 by the papers sent from T. Němec and K. Yasuoka.

#### <u>4.5 Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, Francesca di</u> <u>Mare, D. Addison)</u>

D. Addison presented primary goals and the scope of the paper. The output is to be TGD focused on steam purity, NGC, management, limits and measurements. The first draft has been discussed within the TG and NZ and Japan institutions. There was pointed out, that the purity limits may vary within the countries and

there is a need to find proper consensus. The second draft of the TGD should be prepared by November 2020 and should be available for IAPWS circulation and further development. Full approval is considered for meeting in 2022.

The following discussion:

N. Okita agreed, that the targets/limits for the steam purity are different for Japanese committee and there must be some kind compromise. The discussion should go on by e-mail communication with S. Terada of Japanese PCC representative or on-line meeting.

TÔDO:

The second draft prepared by November 2020 should be circulated in standard IAPWS way. Possibly during May 2021 there should be PCC meeting arranged and the second draft should be there discussed.

- 5. IRS Other Business: No other business.
- IRS Membership: Introduction of new IRS member (proposed by N. Okita and seconded by A. Nový) P. Alberto Giuliano Albo (INRIM - Italy), unanimously accepted by IRS members to be recommended to EC as an IRS member.
- 7. IRS Formal motion to the EC will be prepared by the WG chair
- 8. IRS meeting was adjourned 26. August 2020, about 11:00 (UTC 9:00).

## Agenda for the IAPWS Working Group Industrial Requirements and Solutions (IRS) On-line Meeting, August 26, 2020

- 1. Opening Remarks; Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. Introduction of a new IRS member (P. Alberto Giuliano Albo): incl. in item 6.
- 4. Status of each task of industrial Requirements and Solutions
  - 4.1 Report of the Task Group "Categories of industrial requirements" (<u>N. Okita</u>, chairs or representative of other WG)
  - 4.2 Report of the Task Group "Wet steam properties Calculation" (<u>A. Nový</u>, 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" (<u>S. Senoo</u>, N. Okita, A. Anderko) [Joint with PCAS]
  - 4.4 Report of the joint Task Group on ICRN for acid gas dew points (<u>N. Okita</u>, 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, <u>D. Addison</u>, *S. Terada*) [Joint with PCC] *Note: Names in italic are new task members.*
- 5. Other Business
- 6. Membership
- 7. Preparation of the Formal Motion to the EC
- 8. Adjournment

August 26, 2020 N. Okita (Chair)

## **PCAS WG Minutes**

On-Line (e-mail), July 24 – August 17, 2020

#### 1. About PCAS WG Meeting 2020

IAPWS 2020 meeting in Torino, Italy was canceled and the meeting in Torino is postponed until 2021. PCAS WG Meeting in a face-to-face style was canceled as well and instead, communication about annual matters was held via e-mail. A draft agenda was sent to all PCAS members from Ken Yoshida (chair) on July 24, 2020, and members are requested to make contact with the chair by August 17, 2020, if they have any items that need approval by EC or need to be reported to EC.

#### 2. Adoption of agenda

Agenda has been approved with minor addition of wording.

#### 3. Progress reports on PCAS-related activities

(1) The guideline on self-diffusion coefficients of  $H_2O$  (led by K. Yoshida)

Tasks that are needed for further improvement were examined and assigned to Task Group members after the meeting in Banff last year. Development by individual Task Group members is in progress.

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

IRS WG meeting was virtually held on August 26, 2020, via WebEx. From PCAS, S. Senoo, M. Nakahara, and K. Yoshida attended it. S. Senoo made a presentation about the problems and needs related to wet steam for turbines. Toward bridging the gap between the current situation and the goal of the Task Group, Senoo suggested literature survey to gather and share information among members, in particular about the following three subjects; 1) experimental data in steam turbines, 2) technologies of instrumentation for measurement of droplet size distributions, 3) atomization models. For gathering and sharing related information, Senoo requested attendees and other IAPWS members to send him literature information by March 2021.

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

In the IRS web meeting on August 26, 2020, N. Okita summarized the current status and introduced communication with T. Němec and K. Yasuoka after the last meeting in Banff about related literature.

(4) Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, Francesca di Mare, D. Addison) [in collaboration with IRS and PCC]
In the IRS web meeting on August 26, 2020, and a meeting in Kawasaki, Japan on November 15, 2019, D. Addison presented the goals and scopes of the white paper. From PCAS, S. Senoo, M. Nakahara, and K. Yoshida participated in both of the two meetings and discussed important issues involved in the white paper from the PCAS viewpoints.

#### 4. Possibility of ICRNs

No possible ICRNs have been proposed. Further discussion will be postponed until the meeting in Torino in 2021.

#### 5. International collaboration

No international collaborations have been proposed. Further discussion will be postponed until the meeting in Torino in 2021.

#### 6. Discussion of future activities of PCAS

No future activities have been proposed this year other than those currently in progress. Further discussion will be postponed until the meeting in Torino in 2021.

#### 7. Discussion of the possibility of releases and guidelines

- (1) The guideline on self-diffusion coefficients of H<sub>2</sub>O (led by K. Yoshida) Development will be continued.
- (2) Revision of Revised Release on the Ionization Constant of H<sub>2</sub>O (IAPWS R11-07(2019)) P. Tremaine suggested updating the Revised Release on the Ionization Constant of H<sub>2</sub>O. Tremaine and his co-workers have developed a procedure to derive the self-ionization constant of water from the data of the calibration run on highly pure water with flow conductivity systems. The results obtained by the new procedure are available in J. Phys. Chem. Ref. Data 49, 033103 (2020); https://doi.org/10.1063/1.5127662. The development of the updated version of the IAPWS Release was proposed to include the new data and other data for the high-pressure low temperature region.

#### 8. PCAS membership

No invitation of new members was proposed. Professor Robert H. Wood passed away February 3, 2019.

#### 9. Planning activities for 2020/2021

Each of the activities in Progress Report above will be continued in year 2020/2021.

#### 10. Preparation of report for Executive Meeting

It was confirmed that there are no items needing approval by EC at the virtual meeting on September 11, 2020.

## IAPWS Physical Chemistry of Aqueous Systems (PCAS) Working Group Agenda 2020

- (1) Adoption of agenda
- (2) Appointment of clerk of minutes

Chair would recommend himself, Ken Yoshida, as the clerk of minutes under these abnormal conditions, if there are no other recommendations.

(3) Approval of minutes from the 2019 meeting

The minutes of 2019 PCAS meetings in Banff: http://www.iapws.org/minutes/2019/PCAS2019.pdf The minutes will be approved if there are no corrections nor objections by August 17, 2020.

- (4) Progress reports on PCAS-related activities (by all group members)
- (5) Possibility of ICRNs
- (6) International collaboration
- (7) Discussion of future activities of PCAS
- (8) Discussion of the possibility of releases and guidelines
- (9) PCAS membership
- (10) Planning activities for 2020/2021
- (11) Preparation of report for Executive Meeting

If you have any inputs into items #4 to #11, please send items or documents to Chair (K. Yoshida) by **August 17, 2020**. Regarding #11, an item requiring the approval of EC needs to be sent from WG Chair to the Executive Secretary by August 28, 2020.

July 24, 2020 K. Yoshida (Chair)

#### Czech Society for the Properties of Water and Steam Annual Report 2020

#### Submitted to IAPWS Executive Committee, September 2020

#### Steering board of CZPWS

Chair: Tomáš Němec (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 22, 2020. Due to the covid-19 situation, the form of the meeting was electronic. A significant part of the meeting was devoted to CZPWS funding, in particular to ensuring the membership payments to IAPWS. Payments for 2019 and 2020 are ensured by a national grant led by T. Němec. Despite significant efforts, a long-term funding scheme for IAPWS membership has not yet been ensured.

#### **RESEARCH ACTIVITES**

#### Surface tension of aqueous systems

The research team at the Institute of Thermomechanics of the Czech Academy of Sciences (IT CAS) obtained new data for the surface tension of supercooled water down to -31.4 °C [1,4]. Contrary to previous measurements by Hrubý et al. [J. Phys. Chem. Lett. 5 (2014) 425] and Vinš et al. [J. Phys. Chem. B 119 (2015) 5567], the new data does not refute existence of an anomaly in the temperature trend of surface tension within the deeply supercooled region. An increasing deviation from the IAPWS standard [IAPWS R1-76 (2014)] extrapolated below 0 °C and the new correlation by Pátek et al. [J. Chem. Eng. Data 61 (2016) 928] was detected at temperatures below -25 °C. The motivation for the new experiments carried out with a modified experimental apparatus, allowing for faster measurements at lower temperatures, was to provide an experimental support to the ongoing discussion about the surface tension anomaly, which has been reported recently in several molecular simulations. Possible effect of capillary diameter on the apparent surface tension was studied by R. Mareš and J. Kalová at University of West Bohemia in Pilsen [6].

#### Density of aqueous systems

Accurate measurement of the density of IAPSO Standard Seawater were performed in the supercooled and ambient temperature range (253.15 K to 298.15 K) and from atmospheric pressure to 110 MPa using an in-house developed dual-capillary densimeter (DCD). Complementary measurements were performed from 275.15 K to 343.15 K at atmospheric pressure using commercial vibrating tube densimeter (VTD), which was carefully calibrated [5]. The results were thoroughly compared with the current Release on IAPWS Formulation 2008, IAPWS R13-08. A publication is being prepared. Densities of aqueous systems with ethylene glycol and glycerol under the atmospheric pressure were measured with VTD. Own calibration procedure of VTD based on the work of Fritz et al. [J. Phys. Chem. B 104 (2000) 15] is being developed in order to obtain accurate and reproducible data over wide temperature range. Density of water + glycerol system, including metastable supercooled region, was also investigated using DCD. Currently, the results of measurements are thoroughly analyzed.

#### Cavitation

The problems studied in the SIGMA Research and Development Institute and the Centre of Hydraulic Research in the period June 2019 – May 2020 have been related mainly to the application of models of cavitation erosion during the hydrodynamic cavitation (together with the Institute Physics of the Czech Academy of Sciences) and models of cavitation instabilities in hydrodynamic pumps. In cooperation with IT CAS, the Moscow Power Engineering Institute, the Technical University of Liberec, and the Wuhan University, experimental and numerical modelling of unsteady cavitation phenomena in water has continued in the framework of internal grant projects [2]. In cooperation with IT CAS and the Technical University of Ostrava, experimental and numerical modelling of unsteady multiphase flows has continued, taking into account the interface of water and air [3].

#### Other work

A. Blahut participated in the evaluation of "Release on the IAPWS Formulation 2020 on the Viscosity of Heavy Water".

#### Publications

 Vinš V., Hykl J., Hrubý J., Blahut A., Celný D., Čenský M., Prokopová O.: Possible Anomaly in the Surface Tension of Supercooled Water: New Experiments at Extreme Supercooling down to −31.4 °C, Journal of Physical Chemistry Letters 11 (2020) 4443–4447.

#### **Conference Proceedings**

- 2. Sedlář, M., Krátký, T. and Vyroubal, M.: Numerical modelling of three-dimensional cavitating flow considering thermal and compressibility effects. Proc. EFM 2019, Franzenbad, 2019, to be published in EJP Web of Conf.
- 3. Sedlář, M., Machalka, J. and Komárek, M.: Modeling and optimization of multiphase flow in pump station. Proc. CSMO 2020, Xi'an, 2020, to be published in Journal of Physics.
- 4. Vinš V.: IAPWS Helmholtz Award Lecture Surface Tension of Water, Seawater and Aqueous Binaries at Low Temperatures including Metastable Supercooled Region, IAPWS Symposium Chemistry and Mass Transport for Steam Generation, Banff, Alberta, Canada, October 2, 2019.
- 5. Prokopová O., Blahut A., Čenský M., Vinš V.: Comments on water & air calibration of vibrating-tube densimeter at atmospheric pressure, Proceedings of the int. conf. Experimental Fluid Mechanics 2019, November 19-22, 2020, Franzensbad, Czech Rep. p. 400-407.
- 6. Kalová J., Mareš R., Size dependences of surface tension and measurement accuracy, AIP Conference Proceedings 2189, 020010 (2019)

Attachment 5

## **Report on Activities by INDIAPWS National Committee.**

## Date: 06.08.2020

- 1) A virtual meeting of the Core Committee was conducted on 25.07.2020 from 13.00 hrs to 14.00 hrs and the members have been remotely connected.
- 2) A half day workshop was organized with the support from Mettler Toledo India Pvt. Ltd and WBPDCL (A State PSU Generation co ;) at Kolkata on 10.02.2020. Mr. Kirk Bucher Director (Power) Mettler Toledo-USA gave a presentation on "Importance of Cycle Chemistry Management in Power Plant Operation & Integrity of Equipments. Risk of Grab Sampling and Importance of Online Monitoring for power plant operation with a special reference to IAPWS guidelines on core level instrumentation". The same was attended by approximately 25 participants from different power stations of the eastern part of the country.
- 3) Due to pandemic situation throughout the country and also due to devastating super cyclone at the eastern part of the country the activities of INDIAPWS during the period from March second week to second week July-2020 were slowed down/ became standstill. The proposed workshop during 21.04.2020 to 22.04.2020 could also not be organized.
- 4) A webinar was conducted with special initiative by Shri Amitava Datta on 23.07.2020 in a limited capacity. Participants from NTPC, CGPL-Tata Power & Tata Power-Pryagraj were present. It was a fruitful discussion on recent advances on Power Plant Chemistry management. And the IAPWS TGD3-10 (2015) was also explained in details.
- 5) Since COVID-19 is preventing the travelling of the personnel we have decided to add Webinars in our program schedule; the same will be frequently carried out and it is proposed to conduct a webinar on 13.08.2020 from 15.30 to 17.30 hrs.. The target participants would be from NTPC, Tata power, Semb- Crop and Adani Power & some other IPPs.
- 6) General Members to be included who have shown interests from NTPC, Mettler Toledo (India), SembCorp, Tata Power, Adani Power, Shree Cements, MEIL etc, once the registration and Bank Account is opened within next couple of months.

B.Bhattacharyya. Head Indian National Committee IAPWS

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## Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, September 11, 2020

Japanese National Committee, Chaired by Professor Kenji Yasuoka International Association for the Properties of Water and Steam c/o Japanese Association for the Properties of Water and Steam Chaired by Professor Masaru Nakahara 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: <u>yasuoka@mech.keio.ac.jp</u> URL: https://k-ris.keio.ac.jp/html/100011311\_en.html

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(12) 6691-6698 Mar 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(4) e0231714 10.1371/journal.pone.023171 Apr 2020 4 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. Computational and Structural Biotechnology Journal 18, 1160-1172, 2020

Anisotropy of dodecahedral water cages for guest gas occupancy in semiclathrate hydrates Yuhara, D., Yasuoka, K., Takeya, S., Muromachi, S. Chemical Communications 55(68), 10150-10153 Jan 2019

Cage occupancies, lattice constants, and guest chemical potentials for structure II hydrogen clathrate hydrate from Gibbs ensemble Monte Carlo simulations Brumby, P. E., Yuhara, D., Hasegawa, T., Wu, D. T., Sum, A. K., Yasuoka, K., , Journal of Chemical Physics 150(13) 134503 Apr 2019

Crystal Engineering of Bi2WO6 to Polar Aurivillius-Phase Oxyhalides Morita, K., Park, J. S., Kim, S., Yasuoka, K., Walsh, A. Journal of Physical Chemistry C 123(48) 29155-29161 Dec 2019

Detection of molecular behavior that characterizes systems using a deep learning approach Endo, K., Yuhara, D., Tomobe, K., Yasuoka, K. Nanoscale 11(20) 10064-10071 May 2019

Method to Implement Interaction Surfaces with Virtual Companion Particles for Molecular Dynamics Simulations Koishi, T., Yasuoka, K., Zeng, X. C. Journal of Chemical and Engineering Data 64(9), 3693-3700 Jan 2019

Molecular Dynamic Simulations to Probe Water Permeation Pathways of GPCRs Tomobe, K., Yamamoto, E., Yasuoka, K. Tiberi M. (eds) G Protein-Coupled Receptor Signaling. Methods in Molecular Biology, vol. 1947. Humana Press, New York, NY. Jan 2019

Ordering in clusters of uniaxial anisotropic particles during homogeneous nucleation and growth Nozawa, T., Brumby, P. E., Ayuba, S., Yasuoka, K. Journal of Chemical Physics 150(5) 054903 Feb 2019

Attachment 6

Selectivity of Carbon Nanotubes under An Electric Field on Transferring Water - Alcohol Mixtures Winarto, Yamamoto, E., Yasuoka, K. IOP Conference Series: Materials Science and Engineering 494(1) 012099 Mar 2019

Separation of water-alcohol mixtures using carbon nanotubes under an electric field Winarto, W., Yamamoto, E., Yasuoka, K. Physical Chemistry Chemical Physics 21(28) 15431-15438 Jan 2019

#### Matubayasi, Nobuyuki

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

Solubilization Power of Surfactant-Free Microemulsions Schöttl, S., Matubayasi, N., Horinek, D. Physical Chemistry Chemical Physics 22 10.1039/d0cp02933e 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. Journal of Physical Chemistry B 124(33) 7291-7305 2020

Learning reaction coordinates via cross-entropy minimization: Application to alanine dipeptide Mori, Y., Okazaki, K.-i., Mori, T., Kim, K., Matubayasi, N. The Journal of chemical physics 153(5) 054115 2020

Cavity Particle in Aqueous Solution with a Hydrophobic Solute: Structure, Energetics, and Functionals Zhang, B. W., Matubayasi, N., Levy, R.M. Journal of Physical Chemistry B 124(25) 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. Journal of Colloid and Interface Science 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(3) 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. Journal of Chemical Theory and Computation 16(1) 651-665 2020

Boson peak, elasticity, and glass transition temperature in polymer glasses: Effects of the rigidity of chain bending Tomoshige, N., Mizuno, H., Mori, T., Kim, K., Matubayasi, N. Scientific Reports 9 19514 2019

Local viscoelasticity at resin-metal interface analyzed with spatial-decomposition formula for relaxation modulus Mori, H, Matubayasi, N. The Journal of chemical physics 151(11) 114904 2019

Consistency of geometrical definitions of hydrogen bonds based on the two-dimensional potential of mean force with respect to the time correlation in liquid water over a wide range of temperatures Kikutsuji, T., Kim, K., Matubayasi, N. Journal of Molecular Liquids 294 111603 2019

Bridging the gap between molecular dynamics and hydrodynamics in nanoscale Brownian motions Mizuta, K., Ishii, Y., Kim, K., Matubayasi, N. Soft Matter 15(21) 4380-4390 2019

Diffusion dynamics of supercooled water modeled with the cage-jump motion and hydrogen-bond rearrangement Kikutsuji, T., Kim, K., Matubayasi, N. The Journal of chemical physics 150(20) 204502 2019

Spatially-Decomposed Free Energy of Solvation Based on the Endpoint Density-Functional Method Ishii, Y., Yamamoto, N., Matubayasi, N., Zhang, B. W., Cui, D., Levy, R.M. Journal of Chemical Theory and Computation 15(5) 2896-2912 2019 Free-energy analysis of the hydration and cosolvent effects on the β-sheet aggregation through all-atom molecular dynamics simulation Masutani, K., Yamamori, Y., Kim, K., Matubayasi, N. The Journal of chemical physics 150(14) 145101 2019

Structure and Dynamics of the Hydration Shell: Spatially Decomposed Time Correlation Approach Pluhařová, E., Jungwirth, P., Matubayasi, N., Marsalek, O. Journal of Chemical Theory and Computation 15(2) 803-812 2019

Statistical thermodynamics of regular solutions and solubility parameters Shimizu, S., Matubayasi, N. Journal of Molecular Liquids 273 626-633 2019

The mechanism of salt effects on starch gelatinization from a statistical thermodynamic perspective Nicol, T. W. J., Isobe, N., Clark, J. H., Matubayasi, N., Shimizu, S. Food Hydrocolloids 87 593-601 2 2019

Energetics of cosolvent effect on peptide aggregation Matubayasi, N., Masutani, K. Biophysics and Physicobiology 16 185-195 2019

Energy-representation theory of solutions: Its formulation and application to soft, molecular aggregates Matubayasi, N. Bulletin of the Chemical Society of Japan 92(11) 1910-1927 2019

Spatial-Decomposition Analysis of Electrical Conductivity Matubayasi, N. Chemical Record 19(4) 723-734 2019

#### 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 Self-diffusion of water-cyclohexane mixtures in supercritical conditions as studied by NMR and molecular dynamics simulation. Yoshida K, Nakahara M The Journal of chemical physics 150(17) 174505 May 2019

Handbook of Scientific Tables Nakahara, M., Yoshida K. Maruzen Publishing Co., Ltd., Tokyo and World Scientific Publishing Co, Singapore, in press.

#### Uchida, Hiroshi

Research Scientist, Physical and Chemical Oceanography Research Group, Global Ocean Observation Research Center, Japan Agency for Marine-Earth Science and Technology email: huchida@jamstec.go.jp

An expanded batch-to-batch correction for IAPSO standard seawater Uchida, H.; Kawano, T.; Nakano, T.; Wakita, M.; Tanaka, T.; Tanihara, S. Journal of Atmospheric and Oceanic Technology, 2020, DOI:10.1175/JTECH-D-19-0184.1

Ultra high-resolution seawater density sensor based on a refractive index measurement using the spectroscopic interference method Uchida, H.; Kayukawa, Y.; Maeda, Y. Scientific Reports, 9, 15482, 2019, DOI:10.1038/s41598-019-52020-z

Sensitivity of planktic foraminiferal test bulk density to ocean acidification Iwasaki, S.; Kimoto, K.; Sasaki, O.; Kano, H.; Uchida, H. Scientific Reports, 9, 9803, 2019, DOI:10.1038/s41598-019-46041-x

Japanese effort in the Joint SCOR/IAPSO/IAPWS Committee on the Properties of Seawater (JCS) Uchida, H.; Kayukawa, Y. Kaiyo monthly, 52, 8, 384-389, 2020 (in Japanese, Non-Refereed Paper)

#### Miyamoto, Hiroyuki

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

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., International Journal of Refrigeration, In Press, Journal Pre-proof, 10 July 2020, https://doi.org/10.1016/j.ijrefrig.2020.07.005.

#### Kometani, Noritsugu

Professor, Department of Applied Chemistry & Bioengineering, Graduate School of Engineering, Osaka City University email: kometani@eng.osaka-cu.ac.jp URL: http://www.a-chem.eng.osaka-cu.ac.jp/kometani\_group/index.html

Treatment of Wastewater Containing Persistent Organic Pollutants by Catalytic Hydrothermal Oxidation Method.

Kometani N.

Catalysts & Catalysis 62(3) 173-177 2020

Development of Cu/Ni Binary Catalyst for Hydrothermal Oxidation of Refractory Compounds Kometani N., Narita M. Proc. 12th International Symposium on Supercritical Fluids, OI04 (6 pages) May 2018

Reports on 12th International Symposium on Supercritical Fluids Kometani, N. Rev. High Press. Sci. Technol. 8(3) 227-228 2018

## Mori, Shintaro

Chief researcher, Kurita water industries ltd email: s.mori39@kurita-water.com

Effects on Flow-Accelerated Corrosion of Oleylpropanediamine Under Single-Phase Water Conditions Pertinent to Power Plant Feedwater Weerakul. S., Leaukosol. N., Lister. D. H., Mori. S., Hater. W. CORROSION, 76 (2), 217-230, Feb.2020

## The Swiss National Committee

International Association for the Properties of Water and Steam

#### Report on IAPWS related activities – September 2019 / September 2020 Submitted to the EC Meeting of IAPWS – September 2020

#### **National Committee Contacts:**

President: Marco Lendi, E-mail: marco.lendi@swan.ch Secretary: Tapio Werder, E-mail: tapio.werder@ppchem.com

## Following Institutions 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

#### 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 2021 to find new participating institutions in Switzerland. It was already proposed in Banff, that SCPWS is offering to host the annual IAPWS meeting in Switzerland. Marco Lendi is resigning from Presidency at the end of 2020. New President to be announced later in 2020.

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

M. Lendi, September 2020

### U.S. National Committee to IAPWS 2020 Report on Activities of Potential Interest to IAPWS 9 September 2020

# 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), a new viscosity correlation for heavy water has been developed. A new thermal conductivity correlation (which makes use of the viscosity correlation) has also been completed. These formulations are being evaluated for adoption as IAPWS Releases, and papers have been drafted to be submitted to the *Journal of Physical and Chemical Reference Data*.

A paper was published describing work done in 2019 on the low-density behavior of IAPWS-95, where its virial expansion behaves in unexpected ways near 300 K due to an unphysically large increase in magnitude of the 4th virial coefficient with decreasing temperature. This has implications for attempts to simplify descriptions of fugacity in vapor systems. The publication is: A.H. Harvey, "Anomaly in the Virial Expansion of IAPWS-95 at Low Temperatures," *Int. J. Thermophys.* **40**, 98 (2019).

#### Communicated from OLI Systems, Cedar Knolls, NJ

#### Aqueous chemistry of critical materials

OLI Systems continued working on the aqueous chemistry of rare earth elements under the auspices of DOE's Critical Materials Institute. Recent work has focused on the development of thermodynamic models for (i) the behavior of rare earths in aqueous biological media and (ii) solid-liquid equilibria for rare earth carbonates with emphasis on the precipitation of carbonates as a means for REE recovery. The recent work has been published in the following two papers:

- Y. Fujita, M. Walton, G. Das, A. Dohnalkova, G. Vanzin, and A. Anderko, "Impacts of anthropogenic gadolinium on the activity of the ammonia oxidizing bacterium *Nitrosomonas europaea*," *Chemosphere*, in press, https://doi.org/10.1016/j.chemosphere.2020.127250
- P. Kim, G. Das, M.M. Lencka, A. Anderko, and R.E. Riman, "Precipitation of Rare Earth Carbonates using Monoethanolamine," *Journal of Materials Engineering and Performance*, in press, https://doi.org/10.1007/s11665-020-04887-7

#### Aqueous chemistry for carbon capture and transportation

OLI continued its collaboration with the Institute for Energy Technology (Norway) on the prediction of corrosivity in  $CO_2$  transportation. Recent work was focused on modeling the solubility of nitric and sulfuric acids in carbon dioxide. The acids may form as a result of various reactions between impurities resulting from  $CO_2$  capture processes. The solubility of the acids controls the formation of separate, acid-enriched phases and, therefore, determines the corrosivity of  $CO_2$ -rich phases. The recent work has been published in the paper:

• B.H. Morland, A. Tadesse, G. Svenningsen, R.D. Springer, and A. Anderko, "Nitric and Sulfuric Acid Solubility in Dense Phase CO<sub>2</sub>," *Ind. Eng. Chem. Res.*, 58 (2019) 22924-22933 https://doi.org/10.1021/acs.iecr.9b04957

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

New sound speed measurements in water were reported to 700 MPa from 252 K to 370 K (Bollengier et al., 2019). The methodology and calibration of these ultrasonic determinations were thoroughly documented. In regimes of overlap, the new sound speeds agree at the 100 ppm level with other recent efforts. Augmenting the current work with additional ultrasonic measurements and with sound speeds determined in diamond anvil cells, the full equation of state for water is derived to 2000 MPa and to 500 K. A flexible computational environment of local basis functions (Brown, 2018), allows densities and specific heats to be determined along with statistical maps for their uncertainties as a function of temperature and pressure.

New pressure-temperature-volume determinations at high pressure extending to low temperatures are reported for ice II, III, V, and VI in Journaux et al. (2020). A Gibbs energy representation is generated for each phase based on a quasi-harmonic representation informed by measured or calculated vibrational densities of state. The resulting predictions of solid-solid and solid-liquid phase boundaries are in excellent accord with measurements.

An equation of state of the ice VII-X system is given in Brown and Journaux (2020) that accurately represents pressure-volume-temperature and elastic wave speed measurement to greater than 100 GPa. The representation is sufficiently flexible to assimilate properties through the higher order transitions associated with changes in bonding that are distributed in pressure. Prior representations could either predict properties in limited regimes or had large systematic error when forced to fit measurements over a broader range.

A full open source software and data repository of our work is available through SeaFreeze.org. Tools are provided both in Python and MATLAB programing languages to calculate thermodynamic properties of water and water ices. An app, requiring no user programing, is currently being tested. Other useful software available through SeaFreeze includes a direct MATLAB implementation of the IAPWS-95 representation for water (including an ability to use pressure and temperature as the input) and a separate re-mapping of IAPWS-95 into a Gibbs energy representation that allows greater computational speeds in determination of thermodynamic properties as a function of pressure and temperature.

The cited publications:

- 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 https://doi.org/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

• Brown, J.M., B. Journaux (2020) Local-Basis-Function Equation of State for Ice VII-X to 450 GPa at 300 K, Minerals, 10, 92; doi:10.3390/min1002009

#### Miscellaneous Items

Planning continues for the 21<sup>st</sup> Symposium on Thermophysical Properties to be held on the University of Colorado campus in Boulder, CO, USA from June 20 to 25, 2021. This is part of the triennial series of conferences organized by the Joint ASME-AIChE Committee on Thermophysical Properties. Sessions on Properties of Aqueous Systems will be included in the program. See https://thermosymposium.org/ for current information on the conference. The U.S. Department of Energy continues to sponsor work which could be of interest to IAPWS members; although funding is typically restricted to domestic U.S. entities, some opportunities for collaboration can be found. See https://eere-exchange.energy.gov/Default.aspx for current and recent programs: among the titles are Accelerated Materials R&D, Testing/Qualification, and Cost-Effective Manufacturing Routes for Harsh Service Environments Materials; Research and Development for Advanced Water Resource Recovery Systems; DOE Hydropower Program Research and Development Strategy and HydroWIRES Research Roadmap; and Marine Energy Foundational Research and Testing Infrastructure.

## BRITISH AND IRISH ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

A Member of the International Association for the Properties of Water and Steam



Chair: Mr A. Caswell Vice-Chair: Vacant (applicants received) Secretary: Mr B. Zohm Treasurer: Mr H.W. Lloyd

## BIAPWS ANNUAL REPORT 2020

#### 1 INTRODUCTION

The British and Irish Association for the Properties of Water and Steam (BIAPWS) is the UK and Ireland national committee of the International Association for the Properties of Water and Steam (IAPWS) and the representative body for Power Plant Chemistry in the UK and Ireland. BIAPWS is a not for profit organisation. This is the annual report of the activities of BIAPWS for the period from January 1<sup>st</sup> 2020 to 31<sup>st</sup> August 2020. If you would like to know more about BIAPWS, please feel free to visit our web site www.biapws.org or e-mail BIAPWS at contact.us@biapws.co.uk.

On January 1st I (Adam Caswell) succeeded Mike Sparrey as the BIAPWS chairman.

#### 2 BIAPWS MEMBERSHIP AND MEETINGS

BIAPWS committee meetings are held three times a year and attendance at these continues to be good, typically with around twenty people present. A recent change has been to expand the technical sessions at BIAPWS committee meetings to add value to meeting attendance. Industrial member's representatives are able to bring a colleague to the meetings to benefit from and contribute to the discussions.

This year we held a face to face BIAPWS committee meeting in February. Prior to this we held a survey of our membership to better understand the health and opportunities for BIAPWS, and this was discussed at the meeting. No major changes are planned to BIAPWS, although the following were key learning points from the survey;

1. We intend to encourage new membership from the waste to energy sector, which is growing rapidly in the UK. We will invite new members with reduced or free attendance at upcoming events.

2. We want to re-vamp our website, due to poor functionality and high operating costs.

3. We intend to offer reduced membership rates for small enterprises and retired members, as we feel this is in the best interests of our core ambitions.

4. We intend to host future meetings at varying power plant locations, to encourage diverse attendance and a plant tour element. The first of these was planned for a new nuclear plant currently being constructed, but has been cancelled due to current pandemic restrictions.

Our next meeting will be held virtually in October, when we intend to appoint a new vicechairman, for which we have two applicants. Also, on the agenda are learning from stator chemical cleaning experiences, and upcoming environmental legislation changes.

#### 3 BIAPWS POWER PLANT CHEMISTRY SYMPOSIUM

Each year, BIAPWS organises an annual symposia on power plant chemistry and water treatment. The 21<sup>st</sup> in this series of symposia was planned to be held at the University of Warwick, Coventry, in June 2020.

Unfortunately, we had to cancel this years symposium scheduled in June due to the pandemic. We are progressing our plans for a symposium in the summer of 2021 with caution at present, due to the pandemic restrictions, but are hopeful for an event in some capacity.

#### 4 IAPWS ACTIVITIES

BIAPWS has continued to support IAPWS through its formal membership and participation in IAPWS activities. The support to IAPWS activities is mainly provided directly from those involved, and these are not coordinated or directly tracked through BIAPWS.

#### 5 **BIAPWS AWARDS**

BIAPWS offers selected sponsorship opportunities for student placements and schools events that aim to raise the awareness and generate new interest amongst students in the areas of science and technology relevant to the properties of water and steam, including power plant chemistry. This initiative has in the past proven highly successful, with many previous winners of the BIAPWS Student Award going on to full time employment in power generation.

Over the last 12 months, BIAPWS received no opportunities for sponsorship in 2020.

#### 6 BIAPWS WEBSITE

We currently have plans to re-vamp our website to improve the functionality, and reduce operating costs and complexity. The re-vamp plans will be discussed at the next committee meeting in October, and work is likely to start in early 2021.

#### 7 BSI REPRESENTATION

BIAPWS is currently represented on the three British Standards and Euro Norm Committees listed below of relevance to power plant chemistry and water treatment. However, there have not been any significant developments in recent years.

- PVE/2: Water Tube and Shell Boilers. The UK standards committee has responsibility for BS EN 12952-12:2003: "Water-tube Boilers and Auxiliary Installations - Requirements for Boiler Feedwater and Boiler Water Quality" and BS EN 12953-10:2003: "Shell Boilers -Requirements for Feedwater and Boiler Water Quality".
- CII/62: Treatment of water for boilers. The UK standards committee also has responsibility for BS 2486:1997: "Recommendations for Treatment of Water for Steam Boilers and Water Heaters".
- EH/3/6: Water quality sampling. The UK standards committee is responsible for BS 6068-6.7:1994 (ISO 5667-7:1993): "Guidance on Sampling of Water and Steam in Boiler Plants".

#### 8 INTERACTION WITH PROFESSIONAL ORGANISATIONS

BIAPWS maintains correspondence with a number of professional bodies with the aim of sharing information and closer working.

- BIAPWS is represented on the Energy Sector Interest Group of the Royal Society of Chemistry by John Greene;
- BIAPWS is also represented on the Water Science Forum of the Royal Society of Chemistry by Eric Huff;
- Richard Hill, who is a committee member of the Institution of Chemical Engineers (IChemE) Water Subject Group, is also a Corresponding Member of BIAPWS.

Adam Caswell Chair, British & Irish Association for the Properties of Water and Steam September 20

## German National Committee to IAPWS Executive Committee

## Research Activities on the Thermodynamic Properties of Water and Steam of the German National Committee in the Period 2019/2020

www.iapws.de

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

Vice Chair: Ingo Weber Siemens Power and Gas, Erlangen

#### 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 27th, 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), in press
- 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; <u>https://doi.org/10.3390/e21080799</u> (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; <u>https://doi.org/10.3390/e22010050</u>
- Feistel, R.; Hellmuth, O.: Zur Rolle des Wassers in der Energiebilanz des Klimasystems. Sitzungsberichte der Leibniz-Sozietät zu Berlin, im Druck
- 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. Interfac. Phenom. Heat Transfer 6, 37-74 (2018). DOI: 10.1615/InterfacPhenomHeatTransfer.2018026166
- Hellmuth, O.; Feistel, R.; Foken, T.: Technical Note: Intercomparison of Different State-of-the-Art Formulations of the Mass Density of Humid Air. Atmos. Chem. Phys. (2020), to be submitted.
- Feistel, R.: Thermodynamic Properties of Seawater, Ice and Humid Air: TEOS-10, Before and Beyond. Ocean Sci. 14, 471-502 (2018). <u>https://doi.org/10.5194/os-14-471-2018</u>
- 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). <u>https://doi.org/10.1016/j.pocean.2018.04.004</u>
- Feistel, R.; Lovell-Smith, J. W.: Implementing systematic error in the weight matrix of generalized least-squares regression. published online (2018). <u>https://doi.org/10.13140/RG.2.2.25098.16320</u>

#### 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 firstprinciples calculations.

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

#### **Recent Publications**

o Hellmann, R.:

Reference Values for the Cross Second Virial Coefficients and Dilute Gas Binary Diffusion Coefficients of the Systems  $(H_2O + O_2)$  and  $(H_2O + Air)$  from First Principles. J. Chem. Eng. Data 65, 4130-4141 (2020).  Hellmann, R.; Harvey, A. H.: First-Principles Diffusivity Ratios for Kinetic Isotope Fractionation of Water in Air Geophys. Res. Lett. (2020), DOI: 10.1029/2020GL089999.

 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. (2020), in preparation.

#### Leibniz Institute for Tropospheric Research, Leipzig Dr. Olaf Hellmuth

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

- Feistel, R., F., Hellmuth, O.: Zur Rolle des Wassers in der Energiebilanz des Klimasystems. Sitzungsberichte der Leibniz-Sozietät der Wissenschaften zu Berlin, 144 (2020). In press.
   Feistel, R., F., Hellmuth, O.:
  - On the Role of Water in the Energy Balance of the Climate System. (English translation of the German article "Zur Rolle des Wassers in der Energiebilanz des Klimasystems", Sitzungsberichte der Leibniz-Sozietät der Wissenschaften 144 (2020).
- Foken, T.; Hellmuth, O.; Huwe, B.; Sonntag, D.: Chapter 6: Physical Quantities. In: T. Foken (ed.): Springer Handbook of Atmospheric Measurements. Springer. In press (to be published in 2021).
- Sonntag, D.; Foken, T.; Vömel, H.; Hellmuth, O.: Chapter 9: Humidity Sensors. In: T. Foken (ed.): Springer Handbook of Atmospheric Measurements. Springer. In press (to be published in 2021).
- Görner, Ch.; Franke, J.; Kronenberg, R.; Hellmuth, O.; Bernhofer, Ch.: Multivariate non-parametric Euclidean distance model for hourly disaggregation of daily climate data. Theoretical and Applied Climatology, submitted (under revision).
- Hellmuth, O., Feistel, R., 2020: Analytical determination of the nucleation-prone, low-density fraction of subcooled water. Entropy 2020, 22, 993, doi:10.33909/e22090933 (2020).
- 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. Submitted (2020).
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Real-Gas Effects in Humid Air: Possible Implications of the Advanced Seawater Standard TEOS-10 for Hygrometry at Atmospheric Pressure. Part I: Thermostatic Foundation. Part II: Performance of Enhancement Factor and Relative Fugacity. Wiss. Mitteil. Inst. f. Meteorol. Univ. Leipzig. In preparation.
- Hellmuth, O.; Feistel, R.: Real-Gas Effects in Humid Air: Possible Implications of the Advanced Seawater Standard TEOS-10 for Hygrometry at Atmospheric Pressure. Part III: Effects on Radiative Warming and Cooling in the Water-Vapour Absorption Bands and on the Surface Energy Balance. Wiss. Mitteil. Inst. F. Meteorol. Univ. Leipzig. In preparation.

 Hellmuth, O.; Schmelzer, J. W. P.; Feistel, R.: Ice-crystal nucleation in water: Thermodynamic driving force and surface tension. Part I: theoretical foundation. Entropy, 22, 50, doi:10.3390/e22010050 (2020).

 Hellmuth, O., Schmelzer, J. W. P., Feistel, R.: Ice-crystal nucleation in water: Thermodynamic driving force and surface tension. Part II: verification. In preparation.

### **PPCHEM AG, Hinwil - Switzerland Michael Rziha (Germany)**

Activities

- o New TGD on Air In Leakage (AIL) released and available at the IAPWS homepage
- New TGD on film forming substances (FFS) for industrial plants released and available at the IAPWS homepage.
- New TGD Chemistry Management in Generator Water Cooling during Operation and Shutdown released and available at the IAPWS homepage
- Revision of TGD8-16 on Application of FFS in Fossil, Combined Cycle and Biomass Plants released and available at the IAPWS homepage
- o Ongoing writing of the white paper about FFS application in nuclear plants
- Finalization of the white paper on corrosion product monitoring in flexible (cycling and twoshifting) plants
- o Preparation of the new TGD on Flue Gas Condensation and it's re-use

The elaboration of the white paper on chemistry for geothermal plants is in further progress.

## **Ruhr University Bochum**

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

#### Project:

- 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.

**Recent Publications** 

- o Post, P.; Winhart, B.; di Mare, F.: Large Eddy Simulation of a Condensing Wet Steam Turbine Cascade. J. Eng. Gas Turbines Power, in preparation.
- o 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.
- o 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.
- o Post, P.; Sembritzky, M.; di Mare, F.: Towards scale resolving computations of condensing wet steam flows. ASME Paper GT2019-91269, Proceedings of ASME Turbo Expo 2019: Turbine Technical Conference and Exposition GT2019, June 17 – 21, 2019, Phoenix, Arizona, USA.
- o Iseni, S.; Post, P.; Sembritzky, M.; di Mare, F.: Numerical analysis of the influence of air humidity on a transonic compressor stage. Proceedings of the IGTC 2019 Conference, 17th-22nd November, 2019, Tokyo, Japan.
- o Post, P.; Winhart, B.; di Mare, F.: Large eddy simulation of a condensing flow in a steam turbine cascade. Proceedings of the IGTC 2019 Conference, 17th-22nd November, 2019, Tokyo, Japan.
- o 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.

#### Siemens Power and Gas, Erlangen Ingo Weber

**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.

# STEAG Energy Services, Zwingenberg Dr. Reiner Pawellek, Dr. Tobias Löw

Project

1. Preparation of a fast IAPWS-IF97 property library using SBTL algorithms iteration start values for backward functions.

**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.

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

Projects:

1. The work on the combination of the multi-fluid mixture model with excess Gibbs energy models, especially the predictive model COSMO-SAC, continues. Recently we published an open-source implementation of three different COSMO-SAC models comprising a database of sigma-profiles for about 2262 components including water.

**Recent Publications** 

 Bell, I.H.; Mickoleit, E.; Hsieh, C.-M.; Lin, S.-T.; Vrabec, J.; Breitkopf, C.; Jäger, A. (2020): A Benchmark Open-Source Implementation of COSMO-SAC, J. Chem. Theory Comput. 16(4), 2635–2646.

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

Projects

1. Development of fast property calculation algorithms based on spline interpolation

• The Spline-Based Table Look-Up Method (SBTL) is being applied to the mixture humid air.

2. Application of the developed SBTL method for calculating thermodynamic properties

The developed spline-based property libraries have been implemented into the following process simulation codes:

- Non-stationary thermo-hydraulic code ATHLET of the German Society of Global Research for Safety (GRS), Garching
- Non-stationary thermo-hydraulic code RELAP-7 of the Idaho National Laboratory (INL)
- Process simulation software of Fraunhofer UMSICHT, Oberhausen
- 3. Development of a new ASHRAE standard for calculating thermodynamic properties of moist air, ASHRAE Project SPC-213P.
- 4. Preparation of Chapter 1 for the ASHRAE Handbook of Fundamentals

#### **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.

 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, in preparation.



## New Zealand Association for the Properties of Water and Steam (NZAPWS) Annual Report

Date: 21 September 2020

#### **Key Achievements:**

- 1. NZAPWS is now into its fourth year of full IAPWS membership
- 2. NZAPWS has robust funding in place and has gained additional sponsors for the 2020/2021 year and is in a good financial position
- 3. NZAPWS has an active membership covering the following areas:
  - a. Fossil power generation
  - b. Industrial steam production and use for dairy product production
  - c. Geothermal power generation (subsurface and surface operations)
  - d. Humidity research and services
  - e. Water/steam analytical services
  - f. Water/steam chemical treatment and services
  - g. Electrode/electrical resistance boilers (**Note**: new area of interest for NZ and IAPWS as these plants have started to be installed in NZ to replace existing industrial coal boilers and have presented significant water/steam issues)
- 4. NZAPWS have developed and rolled out a dedicated website <u>www.nzapws.org.nz</u> to provide relevant information and to manage meetings for NZAPWS

#### Key Activities:

1. Due to Covid restrictions we've not held a standard NZAPWS meeting but planning on something, in a shorter format (one day) in December 2020 if conditions allow it

- 2. David Addison has had ongoing involvement in a PCC IAPWS International Collaboration project with the University of New Brunswick (DR Willy Cook) working on high temperature electrochemical corrosion monitoring Covid has prevented any follow up visits to UnB
- 3. David Addison and Ian Richardson have continued working on geothermal related aspects for a IAPWS white paper along with Nobuo Okita (Toshiba) of Japan. A face to face meeting in Tokyo was held in November 2019 between NZAPWS and JAPAWS to discuss key aspects of the draft white paper and the final draft to be issued soon for circulation to PCC/IAPWS
- 4. David Addison has worked on electrode boiler water/steam chemistry issued in conjunction with SIAPWS members (Karsten Thompson and Monica Nielsen) sharing experiences and learnings with various different electrode boiler makes and models
- 5. Jeremy Lovell-Smith is contributing to (a) TPWS via continued investigations into the use of Generalised Least Squares (GLS) to propagate input data covariance into empirical equations, and to (b) JCS through work on the definition of relative humidity.
- Initial planning has commenced for IAPWS 2022 in New Zealand, likely location will be Rotorua in September 2022 to allow attendees to experience the geothermal wonders of New Zealand. No costs have been incurred yet until the Covid situation has stabilized and there is some more clarity. NZAPWS in on standby ready to move on formally going ahead with meeting planning.

## Publications:

None for 2020 at this stage

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