



Australian Association for the Properties of Water and Steam (AUSAPWS) Annual Report

Date: 2 October 2019

Key Achievements:

1. AUSAPWS is in its first year of full membership of IAPWS. Achieved at ICPWS Prague, September 2019.
2. AUSAPWS has established a funding model, and sent a delegate to Banff as part of this model.
3. AUSAPWS now has over 60 members and continues to grow. Our membership primarily covers power generation but has expanded to industrial boilers.

Key Activities:

1. AUSAPWS held out first ever workshop, in April 2019. It was a free seminar held at the AGL Offices in Melbourne.
 - a. 45 Attendees came covering every state in Australia.
 - b. The Workshop was key noted by Michael Rziha and David Addison
 - c. Several key topics in power station chemistry were covered including, FFS, data analytics, cycle chemistry and water treatment.
2. AUSAPWS collaborated with SCIAPWS on the corrosion product monitoring in cycling operations work.
3. Hayden Henderson attended the IAPWS meeting in Banff.
4. AUSAPWS has established a LinkedIn group for discussing of chemistry topics.

AUSAPWS Awards

The AUSAPWS Awards were established to be awarded for services to chemistry in Australia, the first two AUSAPWS awards were awarded to:

- Gary Joy
- David Swainsbury

Publications:

No publications by AUSAPWS members in 2018/2019

Hayden Henderson
AUSAPWS Chairperson
Mobile + 61 499 021 436
Email: hhenderson@agl.com.au

BRITISH AND IRISH ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

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

BIAPWS

www.biapws.org

Chair: Mr. M. Sparrey, ABB Ltd., Oldends Lane, Stonehouse, Gloucestershire, UK
Vice-Chair: vacant
Secretary: Mr B. Zohm, Doosan Babcock, Engineering & Technology, Porterfield Rd, Renfrew, UK
Treasurer: Mr H.W. Lloyd, UK

BIAPWS ANNUAL REPORT 2019

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 August 2018 to July 2019. A list of publications by BIAPWS members during this period is included in Appendix A. 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.

2 BIAPWS MEMBERSHIP AND MEETINGS

BIAPWS membership remains strong, with current support provided by twenty-three industrial sponsors, six honorary members, five ordinary members and eleven corresponding members.

BIAPWS committee meetings are held three times a year and attendance at these continues to be good, typically with around thirty 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.

3 BIAPWS POWER PLANT CHEMISTRY SYMPOSIUM

Each year, BIAPWS organises an annual symposia on power plant chemistry and water treatment. The 20th in this series of symposia was held at the University of Warwick, Coventry, on 29 – 30 May 2019. The symposium consists of introductory sessions on the fundamentals of power plant chemistry and water treatment, followed by more detailed technical presentations. The event remains well supported, with around 90 delegates and 11 exhibition spaces taken up in 2019.

A copy of the symposium programme is included in Appendix B. A paper summarising the proceedings of the 2019 event has been published in Power Plant Chemistry journal.

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4 IAPWS ACTIVITIES

BIAPWS has continued to support IAPWS through its formal membership and participation in IAPWS activities. A number of BIAPWS committee members are represented on IAPWS working groups. At the 2020 IAPWS annual meeting in Kyoto, Japan, BIAPWS will be represented by M. Sparrey BIAPWS Chair and Burkhard Zohm BIAPWS Secretary. In addition, BIAPWS is represented on the executive committee of IAPWS.

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 2018/2019

6 BIAPWS WEBSITE

The public facing pages aim to promote a better understanding of what BIAPWS and IAPWS are and what our activities include. The member's area now includes a library of technical information for our members from BIAPWS meetings and symposia. Further developments are planned to include training resources.

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".

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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.

Mike Sparrey
Chair, British & Irish Association for the Properties of Water and Steam
September 2019

APPENDIX A:

LIST OF UK AND IRELAND ORIGINATED REFERENCE PAPERS IN AREAS OF INTEREST.

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APPENDIX B:

PROGRAMME AND REGISTRATION INFORMATION

20th BIAPWS POWER PLANT CHEMISTRY SYMPOSIUM WEDNESDAY 29th AND THURSDAY 30th MAY 2019 WARWICK CONFERENCES

Scarman Meeting and Conference Centre, Scarman Road, The University
of Warwick, Coventry, CV4 7SH, UK
(see map at end)

PROGRAMME

WEDNESDAY 29TH MAY 2019, 12:00 – 17:00

MANAGEMENT OF COOLING WATER SYSTEMS

12:00 Registration and Lunch - Vendor exhibitions open

13:20 Welcome and introduction

Mike Sparrey, Chair, BIAPWS

13:30 Session 1

Presenters: Biofilm Formation in Water Systems

Katherine Fish, University of
Sheffield

Cooling Water Chemical Treatment

Anthony Matthews, SUEZ

Chair: Eric Huff, Consultant

15:00 Break

15:30 Session 2

Presenters: Life Management of Wooden Cooling
Tower Systems

Phil O'Leary, Exova

Progress with the HSE's Cooling Tower
Intervention Program

Duncan Smith, Health and Safety
Executive

Chair: Eric Huff, Consultant

17:00 Close

19:30 Evening meal, Warwick Conferences

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THURSDAY 30TH MAY 2019, 09:00 – 16:00

POWER PLANT CHEMISTRY AND CORROSION

08:30	Registration and Coffee	
09:00	Welcome and introduction	Mike Sparrey, Chair, BIAPWS
09:05	Exhibitor introductions	Mike Sparrey, Chair, BIAPWS
	Session 1	Chair: Adam Caswell EDF Energy
09:20	Operational Experience of Intermittent Biocide Dosing for Marine Fouling Control	Carl Atkinson, EDF Energy Generation
09:50	Options to Decrease the Scaling Potential and Increase the Recovery Rate of a Reverse Osmosis Process	Uli Dölchow, LANXESS
10:20	Break	
10:50	Assessing the Atmospheric Corrosion Risk for the Storage of Spent Nuclear Fuel at Sizewell B Power Station	Peilong Dong, Imperial College
11:20	Film-Forming Amines for Closed Cooling/Heating Water Systems	Wolfgang Hater, Kurita Europe GmbH
11:50	Open Discussion Session	
12:00	Lunch	

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Session 2		Chair: Paul McCann, Uniper
13:00	Oxide Growth and Exfoliation (OGE) of Superheater and Reheater Tube Materials in Steam	Barry Dooley, Structural Associates
13:30	Field Tests of Proxy Methods for Monitoring Iron Transport at Plants Operating Under Flexible Load Conditions	Karsten Thomsen (COWI) and Maja Skou Jensen (Aarhus University)
14:00	Break	
14:30	Grain CCGT Power Station: Upgrade of Water-Steam Cycle On-Line Monitoring for Flexible Operation	Sarah Gerry, Uniper, Grain Power Station
15:00	Optimisation of the Secondary Circuit Chemical Conditioning at Hinkley Point C	Ruth Oakley and Laurence Vu-Do, EDF
15:30	Open Discussion Session	
15:55	Closing Remarks	Mike Sparrey, Chair, BIAPWS
16:00	Close	

Czech Society for the Properties of Water and Steam Annual Report 2019

Submitted to IAPWS Executive Committee in Banff, Canada, September 30, 2019

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 Meeting

Annual meeting of the CZPWS was held on June 26, 2019. A significant part of the meeting was devoted to CZPWS funding, in particular to ensuring the membership payments to IAPWS. Payment for 2018 has been granted by an anonymous individual. CZPWS expressed its gratitude. Payments for 2019, 2020, and 2021 are ensured by means of an international-cooperation grant by the Czech Ministry of Education, Youth and Sports led by T. Němec. Despite significant efforts, long-term funding of IAPWS membership has not yet been ensured.

Research Activities

Surface tension and density of aqueous systems under supercooled conditions have been investigated at the Institute of Thermomechanics of the Czech Academy of Sciences. The experimental apparatus for the measurement of **surface tension** of supercooled aqueous mixtures [6] has been used to collect new data for the surface tension of seawater [1] and binary aqueous mixtures with sodium chloride and ethylene glycol [7]. The new data for seawater are in good agreement with the correlation by Nayar et al. [J. Phys. Chem. Ref. Data 43 (2014)] extrapolated into the supercooled region down to $-25\text{ }^{\circ}\text{C}$, which is planned to become a new IAPWS standard for the surface tension of seawater. **Density** of cold and supercooled aqueous systems was investigated using a recently developed apparatus enabling high-accuracy density determinations up to pressure of 200 MPa [9]. Density of heavy water has been finalized [2]. Slight differences in isobaric expansivity from values computed from the recent IAPWS formulation (R16-17(2018)) have been found.

The problems studied in the SIGMA Research and Development Institute and the Centre of Hydraulic Research in the period June 2017 – May 2018 have been related mainly to the application of models of cavitation erosion during the hydrodynamic **cavitation** and models of cavitation instabilities to the problems of hydrodynamic pumps [5]. In cooperation with the Institute of Thermomechanics of the Czech Academy of Sciences, 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 been continued in the framework of international grant projects. Recent research is devoted to the influence of real water properties including the content of undissolved air on the pressure pulses excited by cavitation [4].

Thermodynamics of steam with special attention to supersaturated conditions has been studied by molecular simulations using polarizable force fields. Higher virial coefficients have been computed [3] and cluster distributions in steam have been studied [8].

Publications

1. Vinš V., Hykl J., Hrubý J.: *Surface tension of seawater at low temperatures including supercooled region down to $-25\text{ }^{\circ}\text{C}$* , Marine Chemistry 213 (2019) 13-23.
2. Blahut A., Hykl J., Peukert P., Vinš V., Hrubý J.: *Relative density and isobaric expansivity of cold and supercooled heavy water from 254 to 298 K and up to 100 MPa*. J. Chem. Phys. 151 (2019) 034505.

3. Rouha M., Nezbeda I., Hrubý J., Moučka F.: *Higher virial coefficients of water*. J. Mol. Liq. 270 (2018) 81–86.
4. Sedlář, M., Soukal, J., Komárek, M., Volkov, A.V. and Ryzhenkov, A.V.: *Numerical Simulation of Interaction between Fluid and Vapor Structures in Multiphase Flow around Hydrofoil*. J. Appl. Math. Phys., in review.

Conference Presentations

5. Sedlář, M.: *Cavitation phenomena in balancing drums of high-performance feed pumps*. PCC/PCAS/IRS Joint WG Meeting and Workshop, IAPWS Meeting, Kyoto, 2017.
6. Vinš V., Hykl J., Hrubý J., Hošek J., Fransen M., Šmíd B., Nikl Z.: *Seven years of measurement of the surface tension of supercooled water and aqueous mixtures at IT CAS*, 17th International Conference on the Properties of Water and Steam, Prague (Czech Republic), September 2-6, 2018.
7. Vinš V., Hykl J., Čenský M., Hrubý J.: *Surface tension of supercooled aqueous mixtures: Preliminary data for mixtures with alcohols and sodium chloride and for seawater*, 20th Symposium on Thermophysical Properties, Boulder (USA) June 24-29, 2018.
8. Hrubý J., Moučka F., Nezbeda I.: *Cluster distribution and nucleation in steam over a broad temperature range*. 17th International Conference on the Properties of Water and Steam, Prague (Czech Republic), September 2-6, 2018.
9. Blahut A., Duška M., Hykl J., Peukert P., Vinš V., Čenský M., Hrubý J.: *Measurements of density for supercooled ordinary water, heavy water, and seawater at high pressures*. . 17th International Conference on the Properties of Water and Steam, Prague (Czech Republic), September 2-6, 2018.



THE INTERNATIONAL ASSOCIATION FOR
PROPERTIES OF WATER AND STEAM (IAPWS)

**REPORT ON STATUS OF EGYPT'S
NATIONAL COMMITTEE**

Banff 2019

1. Purpose

The purpose of this presentation is to present the activities and plans of Egypt's national committee during 2019 and plans for 2020.

2. Importance of National Committee

- Expansion of Egypt's generating capacity reaching about 80,000 MW (by 2020).
- More than 75 power plants.
- By 2020 Egypt will become in the top 20 list of countries by generating capacity.
- Coal power plants will be added.
- Nuclear Power plants will be added.
- Egypt's national committee will be the channel to international collaboration.
- Opportunity to join forces of national individuals
- To form a national forum to discuss issues and improve performance.
- Platform to define research needs and start a research program to improve capabilities.
- So improving national capacity and capability is essential.

3. Activities in 2019

- Continue to focus with Electric generation sector.
- Prepared an awareness presentations about IAPWS and the initiative of Egypt's national committee.
- Prepared various sessions about some of IAPWS's TGDs
- Prepared application procedures and send to all individual attended seminars.
- Presented many technical presentations about selected IAPWS-TGDs to increase awareness about TGDs in power generation society.
- Maintaining PGESCO support to the initiative.

4. Plans for 2020

- Prepare more seminars at different power plants to allow more people of being involved.
- Prepare more technical sessions about IAPWS's TGDs
- Finalize membership application (some problems).
- Finalize legal form of the NC (still a problem)
- Maintain bank account (after Legal steps)
- Set a communication channel (started)
- Prepare for the 1st meeting.
- Set NC goals and working activities
- Promote in universities and research institutes

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 2018/2019

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 2019 Annual Meeting of the German National Committee took place at Siemens AG Power and Gas Division in Erlangen on 15th March 2019. 24 colleagues attended this meeting. Six papers were presented in the scientific session.

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

Baltic Sea Research Institute, Warnemuende

Dr. Rainer Feistel

Recent Publications

- Feistel, R.:
Distinguishing between Clausius, Boltzmann and Pauling Entropies of Frozen Non-equilibrium States.
Entropy (2019), submitted.
- 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: A Look-up-Table of the TEOS-10 Based Mass Density of Humid Air for Quick-

Look Applications.

Atmos. Chem. Phys. (2019), to be submitted.

- 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>

GFZ German Research Centre for Geosciences

Section 4.8 - Geoenergy

Dr. Harald Milsch, Ulrike Hoffert

Projects

1. Commissioning and optimization of a capillary-type high pressure-high temperature viscometer for aqueous electrolyte solutions at up to 50 MPa and 473 K.
2. Measurements of viscosity of pure and mixed NaCl, CaCl₂, and MgCl₂ aqueous solutions at up to 40 MPa and 353 K.

Publications

- Hoffert, U., Milsch, H.:
A modified flow-through apparatus for high pressure viscosity measurements of salt solutions.
17th International Conference on the Properties of Water and Steam – ICPWS17, Prague, Czech Republic (2018).
- Hoffert, U. and Milsch, H.:
Methods for measuring the density and viscosity of saline geothermal fluids under reservoir conditions.
Proceedings World Geothermal Congress 2020, Reykjavik, Iceland, Paper 13131 (2019).

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.:
Cross second virial coefficient and dilute gas transport properties of the (H₂O + CO₂) system from first-principles calculations.
Fluid Phase Equilib. 485, 251-263 (2019).
- Hellmann, R.:
First-Principles Calculation of the Cross Second Virial Coefficient and the Dilute Gas Shear Viscosity, Thermal Conductivity, and Binary Diffusion Coefficient of the (H₂O + N₂) System.
J. Chem. Eng. Data (2019), submitted.
- 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. (2019), in preparation.

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

Recent Publications (published, submitted, in preparation)

- 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.
- Foken, T.; Hellmuth, O.; Huwe, B.; Sonntag, D.:
Chapter 6: Physical Quantities.
In: T. Foken (ed.): Springer Handbook of Atmospheric Measurements. Springer (in preparation).
Chapter accepted.
- Sonntag, D.; Foken, T.; Vömel, H.; Hellmuth, O.:
Chapter 9: Humidity Sensors.
In: T. Foken (ed.): Springer Handbook of Atmospheric Measurements. Springer (in preparation).
Chapter accepted.

- 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 (2019), submitted.
- Hellmuth, O.; Schmelzer, J. W. P.; Feistel, R.:
Ice-crystal nucleation in water: Thermodynamic driving force and surface tension.
Entropy, Special Issue “Crystallization Thermodynamics” (2019), submitted.
- Hellmuth, O.; Feistel, R.; Foken, T.:
Technical Note: TEOS-10 based mass density for quick-look applications.
Atmos. Chem. Phys. (2019), submitted.
- 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.
In preparation for “Wiss. Mitteil. Inst. f. Meteorol. Univ. Leipzig”.
- 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 II:** Performance of Enhancement Factor and Relative Fugacity.
In preparation for “Wiss. Mitteil. Inst. F. Meteorol. Univ. Leipzig”.
- 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.
In preparation for “Wiss. Mitteil. Inst. F. Meteorol. Univ. Leipzig”.

Ruhr University Bochum

Faculty of Mechanical Engineering, Chair of Thermal Turbomachines and Aeroengines

Prof. Dr. Francesca di Mare

Project:

1. Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the in-house code Shar-C for high-fidelity calculation of unsteady, turbulent flow of condensing steam in low-pressure turbines.
 - The in-house, density-based CFD solver Shar-C accounts for complex thermodynamics, including non-equilibrium condensation and two-phase flow based on tabulation techniques. The two-phase flow is 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. The solver is equipped with a high-resolution, low-dissipation spatial discretization, whilst a 4th – order explicit scheme is employed for time integration. Both a finite-volume and a finite-difference version of the code are available. Classic RANS turbulence models (e.g. k- ω SST, Spalart-Allmaras) as well as scale-resolving models (Wall-Adaptive Large Eddy Simulation) have been implemented and validated. The accuracy of the discretization schemes has

been demonstrated in a Direct Numerical Simulation of decaying, isotropic turbulence also in combination with non-ideal gas properties.

Recent Publications

- Post, P.; di Mare, F.:
Highly efficient Euler-Euler approach for condensing steam flows in turbomachines, GPPS-NA-2018-106.
Proceedings of GPPS Forum 18, Global Power and Propulsion Society, Montreal, 7th-9th May 2018.
- 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.
- Post, P.; di Mare, F.:
Highly efficient Euler-Euler approach with source-term tabulation for condensing wet steam flows.
Proceedings of the 2nd International Workshop on non-ideal compressible fluid dynamics (NICFD2018), Bochum, Germany, 4th-5th October, 2018.
- 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.
- 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.
- 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.

Ruhr University Bochum**Faculty of Mechanical Engineering, Chair of Thermodynamics****Prof. Dr. Roland Span**

Projects:

1. The work on the new reference equation of state for heavy water (D₂O) has been completed. The release published in 2017 has been revised to account for the last changes. The revised release was adopted by IAPWS on the 2018 annual meeting and was subsequently published on the IAPWS website (<http://www.iapws.org/relguide/Heavy.html>). Details on the new equation of state were published in the Journal of Physical and Chemical Reference Data.
2. The work on a new mixed gas hydrate model consistent to reference equations of state comes into its final phase. This work started as a collaboration of Ruhr University Bochum (Prof. Dr. Roland Span, Dr. Andreas Jäger) and the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš). The work is now carried on as a collaboration of Ruhr University Bochum (Prof. Dr. Roland Span, Dr. Sebastian Hielscher), the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš), and TU Dresden (Prof. Dr. Cornelia Breitung, Dr. Andreas Jäger). Recently, Dr. Sebastian Hielscher was promoted Dr.-Ing. based on his work on hydrates. Further work will likely address hydrogen hydrates and hydrate types that are stable only in mixed hydrates.

Recent Publications

- Herrig, S.; Thol, M.; Harvey, A. H.; Lemmon, E. W.:
A Reference Equation of State for Heavy Water,
J. Phys. Chem. Ref. Data 47, 043102 (2018).
- Hielscher, S.; Semrau, B.; Jäger, A.; Vinš, V.; Breitung, C.; Hrubý, J.; Span, R.:
Modification of a model for mixed hydrates to represent double cage occupancy,
Fluid Phase Equilibria 490, 48-60 (2019).

Ruhr University Bochum

Faculty of Mechanical Engineering, Chair of Thermodynamics

Prof. em. Dr. Dr. e. h. Wolfgang Wagner

Project

1. Completion of the 3rd edition of the book "International Steam Tables".
2. Preparation of the Chapter "Thermophysikalische Stoffwerte von Wasser (Thermophysical properties of Water)" for the VDI-Wärmeatlas (VDI-Heat Atlas) 2018.

Recent Publications

- Kretzschmar, H.-J.; Wagner, W.:
International Steam Tables – Properties of Water and Steam based on the Industrial Formulation IAPWS-IF97.
Springer-Verlag, Berlin (2019).
- Kretzschmar, H.-J.; Wagner, W.:
Thermophysikalische Stoffwerte von Wasser.
In: P. Stephan et al. (Hrsg.), Springer Reference Technik, VDI-Wärmeatlas, 12. Auflage. VDI Springer Reference (2019).
- 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 / PPCHEM AG

Michael Rziha

Activities

- New TGD on Air In Leakage (AIL)
- New TGD on film forming substances (FFS) for industrial plants.
- New TGD Chemistry Management in Generator Water Cooling during Operation and Shutdown
- Revision of TGD8-16 on Application of FFS in Fossil, Combined Cycle and Biomass Plants

Beside that also white papers are in preparation with the perspective becoming in near future also a TGD. Those are in particular a white paper about FFS application in nuclear plants and a white paper about corrosion product sampling and monitoring for cycling plant. This white on corrosion product monitoring was also part of the international collaboration, which was and is excellently progressing with important results.

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

With respect to promoting IAPWS, there had been numerous activities and events recently making IAPWS more and more known to the entire world. Just a few highlights:

- The 3rd IAPWS conference on FFS in Heidelberg this year was a great success with increasing number of participants (attracted more than 70 participants from 22 countries)
- The 6th IAPWS conference EHF (European HRSG Forum) in Athens was also extremely well visited, also with more than 70 participants from around the globe. Straight after this EHF a 1 day symposium of the "re-animated" Greek IAPWS (HIAPWS) was held and also this was a real highlight, since the HIAPWS seems now coming really back to the scene and showed a strong willingness and motivation to do that.
- Australia and New Zealand had also organized very successful meetings this year. In both events around 50 participants from each country had been present and both events demonstrated a great motivation and interest for a stronger and intensive collaboration with IAPWS. Also in both events it was demonstrated that the IAPWS TGD have taken over a leading role as the number 1 reference and guiding documents for all power plant chemistry applications and questions.
- Another superb example for the leading role of IAPWS and the TGD of PCC are that the IEC have withdrawn their standard on steam purity (which was in place since many decades) in favor of the IAPWS TGD 5-13 and so this TGD is now THE worldwide standard on steam purity for all kind of turbines.

Projects

Development of new Technical Guidance Documents:

1. FFS in Industrial Plants – Release in Banff 2019
2. Chemistry Management in Generator Water Cooling – Release in Banff 2019
3. Film Forming Substances (FFS) for Nuclear Plants – "White Paper is in preparation"
4. Demin Water Integrity – Final Draft will be discussed in Banff, 2019.
5. Corrosion product (CP) sampling and analysing – "White Paper" is in preparation. Excellent results by Int. Collaboration gained so far and those will be integrated into this white paper.
6. Chemistry in Geothermal Plant – "White Paper" will be introduced in Banff

Siemens Power and Gas, Erlangen

Ingo Weber

Projects

1. Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code KRAWAL
 - The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the heat cycle code KRAWAL which is used worldwide by Siemens.
 - The computing time consumption of KRAWAL has been significantly reduced.

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. Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code EBSILON
 - The “IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)” has been implemented into the heat cycle code EBSILON which is used worldwide by the power industry.
 - The computing time consumption of EBSILON has been significantly reduced.

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 a new model for mixed gas hydrates continues. This work started as a collaboration of Ruhr-Universität Bochum (Prof. Dr. Roland Span, Dr. Andreas Jäger) and the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš). The work is now carried on as a collaboration of Ruhr-Universität Bochum (Prof. Dr. Roland Span, Sebastian Hielscher), the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš), and TU Dresden (Prof. Dr. Cornelia Breitkopf, Dr. Andreas Jäger). The model for CCS-relevant mixed hydrates has been modified in a way that double occupancy is now also taken into account. This resulted in a publication by Hielscher et al. (2019).

2. The multi-fluid mixture model was combined with different versions of the predictive excess Gibbs energy model COSMO-SAC [Jäger et al. (2019)]. Results of the new model for water have been presented on the 17th ICPWS in Prague (2018).
3. Molecular simulations of volumetric properties and cage occupancies of gas hydrates in different crystal structures have been conducted and are ongoing work (Dr. Tommy Lorenz, Dr. Andreas Jäger). Properties of gas hydrate formers in structures that these hydrate formers do not form, if they are in a binary mixture with water, are important for the development of a model for mixed hydrates. As these quantities cannot be obtained experimentally, simulations are a viable option. First results will be presented on the 17th ICPWS in Prague (2018). A paper is in preparation.

Recent Publications

- Hielscher, S.; Semrau, B.; Jäger, A.; Vinš, V.; Bretkopf, C.; Hrubý, J.; Span, R.:
Modification of a model for mixed hydrates to represent double cage occupancy.
Fluid Phase Equilib. 490, 48-60 (2019).
- Jäger, A.; Mickoleit, E.; Bretkopf, C.:
A combination of multi-fluid mixture models with COSMO-SAC.
Fluid Phase Equilib. 476, 147-156 (2018).

University of Rostock, Rostock

Institute of Chemistry, Chair of Technical Thermodynamics

Dr. Javid Safarov

Project

1. Thermophysical Properties of Sea- and geothermal waters, aqueous salt solutions
Thermophysical Properties of Sea- and geothermal waters, aqueous salt solutions, seawater over a wide range of temperatures, pressures and concentration were reported.
An equation of state (EOS) for fitting of the (p, ρ, T) data has been developed as a function of pressure, temperature and molality. Various thermophysical properties were calculated.

Recent Publications

- Mirzaliyev, A.; Safarov, J.; Hassel, E.:
Thermophysical properties of Thessaloniki Aegean seawater.
Journal of Scientific Works of Azerbaijan Technical University 4, 30-36 (2018).
- Mirzaliyev, A.; Safarov, J.; Hassel, E.:
Viscosity of the Caspian Seawater.
Journal of Scientific Works of Azerbaijan Technical University 2, 39-45 (2018).
- Ziraman, D. U.; Safarov, J. T.; Doğan, Ö. M.; Hassel, E. P.; Uysal, B. Z.:
Apparent molar volumes V_ϕ of calcium acetate $(\text{Ca}(\text{CH}_3\text{COO})_2 (\text{aq}))$ at $T=(273.15 \text{ to } 353.15) \text{ K}$ and pressures up to 100 MPa.
Journal of the Serbian Chemical Society 83, 1005-1016 (2018).
- Mirzaliyev, A.; Safarov, J.; Hassel, E.:
Chemical and thermophysical properties of Bosphorus Seawater.
“Transactions” of Pedagogical University of Azerbaijan. Mathematical and Natural Sciences Series 2, 67-75 (2018).

- Talibov, M. A.; Safarov, J. T., Hassel, E.; Abdulagatov, I. M.:
High-Pressure and High-Temperature Density and Vapor-Pressure Measurements and Derived Thermodynamic Properties of Natural Waters of Yardimli District of Azerbaijan.
High Temperature – High Pressure 47, 223-255 (2018).
- Ahmadov, A.; Safarov, J.; Bashirov, M.; Hassel, E.:
Density of geothermal energy resources of Gabala region of Azerbaijan at high pressures and wide range of temperatures.
Monitoring, Science and technology (*Nauka i texnologiya*), Maxachkala, Russian Federation 4, 56-61 (2017).
- Gilbert, W. J. R.; Safarov, J.; Minnick, D. L.; Rocha, M. A.; Hassel, E.; Shiflett, M.:
Density, Viscosity, and Vapor Pressure Measurements of Water + Lithium bis(trifluoromethylsulfonyl) imide Solutions.
J. Chem. Eng. Data 62, 2056-2066 (2017).
- Safarov, J.; Mammadova, E.; Shahverdiyev, A.; Hassel, E.:
Thermodynamic properties of the Arkivan-Seyfeddin (Masalli, Azerbaijan) geothermal water.
Monitoring, Science and technology (*Nauka i texnologiya*), Maxachkala, Russian Federation 2, 82-91 (2017).

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)
 - Heat-cycle simulation software KRAWAL of Siemens Power and Gas, Erlangen
 - Heat-cycle simulation software EBSILON of STEAG Energy Services, Zwingenberg
 - Process simulation software of Fraunhofer UMSICHT, Oberhausen

3. Development of algorithms for the transport properties of moist air, ASHRAE Research Project RP-1767.
4. Development of a new ASHRAE standard for calculating thermodynamic properties of moist air, ASHRAE Project SPC-213P.
5. Completion of the 3rd edition of the book "International Steam Tables".
6. Preparation of the Chapter "Thermophysikalische Stoffwerte von Wasser (Thermophysical properties of Water)" for the VDI-Wärmeatlas (VDI-Heat Atlas) 2018
7. Preparation of Chapter 1 for the ASHRAE Handbook of Fundamentals

Recent Publications

- Kretzschmar, H.-J.; Wagner, W.:
International Steam Tables – Properties of Water and Steam based on the Industrial Formulation IAPWS-IF97.
Springer-Verlag, Berlin (2019).
- Kretzschmar, H.-J.; Wagner, W.:
Thermophysikalische Stoffwerte von Wasser.
In: P. Stephan et al. (Hrsg.), Springer Reference Technik, VDI-Wärmeatlas, 12. Auflage.
VDI Springer Reference (2019).
- Kunick, M.:
Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL).
Fortschritt-Bericht VDI, Reihe 6, Energietechnik, Nr. 618 (2018).
- Herrmann, S.; Kretzschmar, H.-J.; Aute, V. C.; Gatley, D. P.; Vogel, E.:
Transport Properties of Real Moist Air, Dry Air, Steam, and Water.
Report ASHRAE RP-1767, ASHRAE, Atlanta, GA (2019).
- Kretzschmar, H.-J.; Herrmann, S.; Schneider, M.; Jaehne, I.:
Learning System Thermopr@ctice for the Calculation of Exercises with Mathcad.
In: Proceedings of the Congress INFORINO, Trudi Mehdunarodny Nauchno-Metodichesky Konferenzy, Isdatjelstvo, Moscow Power Engineering Institute, Moskva (2018).
- Herrmann, S.; Vogel, E.:
New Formulation for the Viscosity of n-Butane.
J. Phys. Chem. Ref. Data 47, 013104 (2018).
- Herrmann, S.; Hellmann, R.; Vogel, E.:
Update: Reference Correlation for the Viscosity of Ethane [J. Phys. Chem. Ref. Data 44, 043101 (2015)].
J. Phys. Chem. Ref. Data 47, 023103 (2018).
- 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.

**Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS,
Banff, Canada, September–October 2019**

**Japanese National Committee, Chaired by Professor Kenji Yasuoka
International Association for the Properties of Water and Steam
c/o The 139th Committee on Steam Properties
Japan Society for the Promotion of Science (JSPS),
Chaired by Professor Masaru Nakahara
5-3-1, Kojimachi, Chiyoda-ku
Tokyo 102-0083, Japan**

I. Overview:

The Japan National Committee, supported by JSPS, 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. Since we organized IAPWS Annual Meetings in 2017, we have further promoted international cooperation as can be seen in minutes and documents at the IAPWS website. Some of our members are active as the members of the IAPWS Working Groups and making efforts in each working group. 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:

Nakahara, Masaru

Professor Emeritus of Kyoto University, Institute for Chemical Research
email: nakahara@scl.kyoto-u.ac.jp

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.

Yasuoka, Kenji

Professor, Department of Mechanical Engineering, Keio University

email: yasuoka@mech.keio.ac.jp

URL: <http://www.yasuoka.mech.keio.ac.jp>

Cage occupancies, lattice constants, and guest chemical potentials for structure II hydrogen clathrate hydrate from Gibbs ensemble Monte Carlo simulations

Brumby P., Yuhara D., Hasegawa T., Wu D., Sum A., Yasuoka K.
Journal of Chemical Physics 150(13) Apr 2019

Ordering in clusters of uniaxial anisotropic particles during homogeneous nucleation and growth

Nozawa T., Brumby P., Ayuba S., Yasuoka K.
Journal of Chemical Physics 150(5) Feb 2019

A fast and accurate computational method for the linear-combination-based isotropic periodic sum

Takahashi K., Nozawa T., Yasuoka K.
Scientific Reports 8(1) Dec 2018

Effect of central longitudinal dipole interactions on chiral liquid-crystal phases

Nozawa T., Brumby P., Yasuoka K.
International Journal of Molecular Sciences 19(9) Sep 2018

Molecular Dynamics Simulation of Ice Crystal Growth Inhibition by Hexadecyl-trimethyl-ammonium Bromide

Shimazu N., Takaiwa D., Suh D., Kawaguchi T., Fuse T., Kaneko T., Yasuoka K.
Langmuir 34(31) 9330-9335 Aug 2018

Kinetic analysis of homogeneous droplet nucleation using large-scale molecular dynamics simulations

Ayuba S., Suh D., Nomura K., Ebisuzaki T., Yasuoka K.
Journal of Chemical Physics 149(4) Jul 2018

Phase behaviors of deeply supercooled bilayer water unseen in bulk water

Kaneko, T., Bali J., Akimoto T., Francisco J. S., Yasuoka K., and Zeng X. C.
Proceedings of the National Academy of Sciences of USA 115(19) 4839-4844 May 2018

Analysis of three-phase equilibrium conditions for methane hydrate by isometric-isothermal molecular dynamics simulations

Yuhara, D., Brumby, P. E., Wu, D., Sum, A. K., Yasuoka, K.
J. Chem. Phys. 148(18) 184501 (9 pages) May 2018

Density functional theory study of atomic and electronic properties of defects in reduced anatase TiO₂ nanocrystals

Morita K., Yasuoka K.
AIP Advances 8(3) 035119 (14 pages) Mar 2018

Detection of Anomalous Dynamics for a Single Water Molecule

Tomobe, K., Yasuoka, K.
J. Chem. Theory Comput. 14(3) 1177-1185 Mar 2018

Critical test of isotropic periodic sum techniques with group-based cut-off schemes

Nozawa, T., Yasuoka, K., Takahashi, K. Z.
Scientific Reports 8(1) 4185 (9 pages) Mar 2018

Heterogeneous cavitation and crystallisation with an impurity by molecular dynamics

Suh, D., and Yasuoka, K.
Molec. Simul. 44(7) 530-533 Mar 2018

Structural determinants in the bulk heterojunction

Acocella, A., Hofinger, S., Haunshmid, E., Pop, C., S., Narumi, T., Yasuoka, K., Yasui, M., Zerbetto, F.
Phys. Chem. Chem. Phys. 20(8) 5708-5720 Feb 2018

Multi-step time series generator for molecular dynamics

Endo K., Tomobe K., Yasuoka K.
32nd AAAI Conference on Artificial Intelligence, AAAI 2018 2192-2199 2018

Oxygen vacancy-originated highly active electrocatalysts for the oxygen evolution reaction

Hirai S., Morita K., Yasuoka K., Shibuya T., Tojo Y., Kamihara Y., Miura A., Suzuki H., Ohno T., Matsuda T., Yagi S.
Journal of Materials Chemistry A 6(31) 15102-15109 2018

Recent advances in clathrate hydrates research using molecular simulations

Yuhara D., Hiratsuka M., Yasuoka K.
Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu 28(2) 102-112 2018

Self-assembly of peptide amphiphiles by vapor pressure osmometry and dissipative particle dynamics

Seki T., Arai N., Suh D., Ozawa T., Shimada T., Yasuoka K., Hotta A.
RSC Advances 8(47) 26461-26468 2018

Theoretical analyses on water cluster structures in polymer electrolyte membrane by using dissipative particle dynamics simulations with fragment molecular orbital based effective parameters

Okuwaki K., Mochizuki Y., Doi H., Kawada S., Ozawa T., Yasuoka K.
RSC Advances 8(60) 34582-34595 2018

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

High-Pressure and High-Temperature NMR Observation of Synthetic Polymers: High-Resolution Measurement Taking Advantage of Motional Narrowing in Sub-Critical Fluids

Tomohiro Hirano, Ken Yoshida, Miyuki Oshimura, Koichi Ute

The Review of High Pressure Science and Technology Vol.28(No.2) 95-101 Jul 2018

Chronological Scientific Tables 2019

Yoshida K.

pp.513-520, 525-528, Maruzen Publishing Co., Ltd., Tokyo, ISBN 978-4621302187 Nov 2018

Handbook of Scientific Tables

Nakahara, M., Yoshida K.

Maruzen Publishing Co., Ltd., Tokyo and World Scientific Publishing Co, Singapore, in press.

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>

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 Sep 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

J. Mol. Liq. 294 111603 Sep 2019

Spatially-Decomposed Free Energy of Solvation Based on the Endpoint Density-Functional Method.

Ishii Y, Yamamoto N, Matubayasi N, Zhang BW, Cui D, Levy RM

Journal of chemical theory and computation 15(5) 2896-2912 May 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 May 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 May 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 Apr 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 Feb 2019

The mechanism of salt effects on starch gelatinization from a statistical thermodynamic perspective

Nicol Thomas W. J., Isobe Noriyuki, Clark James H., Matubayasi Nobuyuki, Shimizu Seishi

FOOD HYDROCOLLOIDS 87 593-601 Feb 2019

Refining evERdock: Improved selection of good protein-protein complex models achieved by MD optimization and use of multiple conformations

Shinobu Ai, Takemura Kazuhiro, Matubayasi Nobuyuki, Kitao Akio

JOURNAL OF CHEMICAL PHYSICS 149(19) 195101 Nov 2018

Statistical thermodynamics of regular solutions and solubility parameters

Matubayasi Nobuyuki, Shimizu Seishi

J. Mol. Liq. 273 626-633 Oct 2018

Spatial-Decomposition Analysis of Electrical Conductivity.

Matubayasi N

Chemical record (New York, N.Y.) Oct 2018

Resin filling into nano-sized pore on metal surface analyzed by all-atom molecular dynamics simulation over a variety of resin and pore sizes

Mori Hodaka, Matubayasi Nobuyuki

POLYMER 150 360-370 Aug 2018

Free-energy analysis of physisorption on solid-liquid interface with the solution theory in the energy representation

Yamamoto Naoki, Nakakuki Ippei, Matubayasi Nobuyuki

JOURNAL OF CHEMICAL PHYSICS 149(1) 014504 Jul 2018

How do hydrogen bonds break in supercooled water?: Detecting pathways not going through saddle point of two-dimensional potential of mean force

Kikutsuji Takuma, Kim Kang, Matubayasi Nobuyuki

JOURNAL OF CHEMICAL PHYSICS 148(24) 244501 Jun 2018

Structure and permeability of ionomers studied by atomistic molecular simulation combined with the theory of solutions in the energy representation

Kawakami Tomonori, Shigemoto Isamu, Matubayasi Nobuyuki
JOURNAL OF CHEMICAL PHYSICS 148(21) 214903 Jun 2018

Statistical thermodynamic foundation for mesoscale aggregation in ternary mixtures

Shimizu Seishi, Matubayasi Nobuyuki
PHYSICAL CHEMISTRY CHEMICAL PHYSICS 20(20) 13777-13784 May 2018

The Excess Chemical Potential of Water at the Interface with a Protein from End Point Simulations

Zhang Bin W., Cui Di, Matubayasi Nobuyuki, Levy Ronald M.
JOURNAL OF PHYSICAL CHEMISTRY B 122(17) 4700-4707 May 2018

Free-Energy Analysis of Peptide Binding in Lipid Membrane Using All-Atom Molecular Dynamics Simulation Combined with Theory of Solutions

Mizuguchi Tomoko, Matubayasi Nobuyuki
JOURNAL OF PHYSICAL CHEMISTRY B 122(13) 3219-3229 Apr 2018

Probabilistic analysis for identifying the driving force of protein folding

Tokunaga Yoshihiko, Yamamori Yu, Matubayasi Nobuyuki
JOURNAL OF CHEMICAL PHYSICS 148(12) Mar 2018

Binding free energy analysis of protein-protein docking model structures by evERdock

Takemura Kazuhiro, Matubayasi Nobuyuki, Kitao Akio
JOURNAL OF CHEMICAL PHYSICS 148(10) Mar 2018

Spatial-decomposition analysis of viscosity with application to Lennard-Jones fluid

Tu Kai-Min, Kim Kang, Matubayasi Nobuyuki
JOURNAL OF CHEMICAL PHYSICS 148(9) Mar 2018

Ion hydration: linking self-diffusion and reorientational motion to water structure

Shimizu Seishi, Matubayasi Nobuyuki
PHYSICAL CHEMISTRY CHEMICAL PHYSICS 20(8) 5909-5917 Feb 2018

A unified perspective on preferential solvation and adsorption based on inhomogeneous solvation theory

Shimizu Seishi, Matubayasi Nobuyuki
PHYSICA A-STATISTICAL MECHANICS AND ITS APPLICATIONS 492 1988-1996 Feb 2018

The Role of Interfacial Water in Protein-Ligand Binding: Insights from the Indirect Solvent Mediated Potential of Mean Force

Cui Di, Zhang Bin W., Matubayasi Nobuyuki, Levy Ronald M.
JOURNAL OF CHEMICAL THEORY AND COMPUTATION 14(2) 512-526 Feb 2018

MD simulation analysis of resin filling into nano-sized pore formed on metal surface

Mori Hodaka, Matubayasi Nobuyuki

APPLIED SURFACE SCIENCE 427 1084-1091 Jan 2018

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

Global observing needs in the deep ocean

Levin, L. A. et al.

Frontiers in Marine Science, 6:241, 2019, DOI:10.3389/fmars.2019.00241

WHP P17E Revisit in 2017 Data Book

Uchida, H.; Murata, A.; Harada, N.; Doi, T.

Published by Japan Agency for Marine-Earth Science and Technology, 2019, DOI:10.17596/0000003

Compact underwater slip ring swivel: Minimizing effect of CTD package rotation on data quality

Uchida, H.; Maeda, Y.; Kawamata, S.

Sea Technology, 11, 30-32, 2018.

Hadal water biogeochemistry over the Izu-Ogasawara Trench observed with a full-depth CTD-CMS

Kawagucci, S.; Makabe, A.; Kodama, T.; Matsui, Y.; Yoshikawa, C.; Ono, E.; Wakita, M.; Nunoura, T.; Uchida, H.; Yokokawa, T.

Ocean Science, 14, 575-588, 2018. DOI:10.5194/os-14-575-2018

Estimates of methane emissions from the Southern Ocean from quasi-continuous underway measurements of the partial pressure of methane in surface seawater during the 2012/13 austral summer

Oanh Thi Ngoc Bui; Kameyama, S.; Yoshikawa-Inoue, H.; Ishii, M.; Sasano, D.; Uchida, H.; Tsunogai, U.

Tellus B, 70, 1-15, 2018. DOI:10.1080/16000889.2018.1478594

Hirano, Hideo

Retired Senior Research Scientist, Central Research Institute of Electric Power Industry

email: hhirano0879@jcom.home.ne.jp

Trend of the Water Conditioning for Boiler Water : Overview of low-concentration sodium hydroxide treatment (In Japanese).

Hirano, H., Shimokado, T., Kamizasa, M., Yoshida M.

Boiler yearbook, 2018 edition, Japan Boiler Association, pp. 40-49 (November 2018).

PWR secondary water chemistry guidelines in Japan - Purpose and technical background.
Kawamura, H; Shoda, Y; Terachi, T; Katsumura, Y; Uchida, S; Mizuno, T; Muroya, Y;
Tsuzuki, Y; Umehara, R; Hirano, H; Nishimura, T;
Progress in Nuclear Energy, Vol. 114, July 2019, pp 121-137

Okazaki, Susumu

Professor, Department of Materials Chemistry, Nagoya University
email:okazaki@apchem.nagoya-u.ac.jp,
URL: <http://simulo.apchem.nagoya-u.ac.jp/index.html>

Molecular mechanism of material deformation and failure in butadiene rubber: Insight from all-atom molecular dynamics simulation using a bond breaking potential model
Payal R.S., Fujimoto K., Jang C., Shinoda W., Takei Y., Shima H., Tsunoda K., Okazaki S.
POLYMER 170 113-119 Apr 2019

All-atom molecular dynamics study on the non-solvent induced phase separation: Thermodynamics of adding water to poly(vinylidene fluoride)/N-methyl-2-pyrrolidone solution
Taddese T., Kitabata M., Okazaki S.
JOURNAL OF CHEMICAL PHYSICS 150(18) 184505 May 2019

Molecular Dynamics of Polyrotaxane in Solution Investigated by Quasi-Elastic Neutron Scattering and Molecular Dynamics Simulation: Sliding Motion of Rings on Polymer
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POLYMER 178 Sep 2019

Adschiri, Tadafumi

Professor, Wpi- AIMR, Tohoku University

email: tadafumi.ajiri.b1@tohoku.ac.jp

URL: http://www.wpi-aimr.tohoku.ac.jp/ajiri_lab/

Atomic-Scale Valence State Distribution inside Ultrafine CeO₂ Nanocubes and Its Size Dependence

XD.Hao, A.Yoko, CL.Chen,K.Inoue, M.Saito, GY.Seong, S.Takami, T.Adschiri, Y.Ikuhara

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Tsuchiya, Noriyoshi

Graduate School of Environmental Studies, Tohoku University

email: tsuchiya@mail.kankyotohoku.ac.jp

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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

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Uchida, Shunsuke

Research consultant, Reactor Safety Research Center, Japan Atomic Energy Agency
email: uchida.shunsuke@jaea.go.jp

Improvement of plant reliability based on combination of prediction and inspection on crack growth due to intergranular stress corrosion cracking

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The corrosion of aluminum alloy in containment after a loss-of-coolant accident

Huang J., Lister D., Uchida S., Liu L.

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NEW ZEALAND
Association for the Properties of
WATER & STEAM



Tō AOTEAROA
Ranga mō ngā Āhuatanga o te
WAI ME TE MAMAOA

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

Date: 27 September 2019

Key Achievements:

4. NZAPWS is now into its third year of full IAPWS membership
5. NZAPWS has robust funding in place and has gained additional sponsors for the 2019/2020 year and is in a good financial position
6. 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
7. NZAPWS have developed and rolled out a dedicated website – www.nzapws.org.nz to provide relevant information and to manage meetings for NZAPWS

Key Activities:

1. A very successful technical seminar was held in May 2019 in Rotorua, NZ with 50 attendees and a wide ranging program of technical presentations covering;
 - a. Geothermal steam chemistry
 - b. Industrial steam chemistry
 - c. Humidity
 - d. Water and steam chemical analysis
 - e. Cooling water systems
 - f. Steam heat transfer
 - g. IAPWS related research and Technical Guidance Documents

The 2-day seminar was based on NZAPWS member demands and included a NZAPWS networking dinner with the seminar fostering knowledge sharing and collaboration between different water/steam users, vendors

Michael Rziha from PPChem attended and presented on the activities of PCC and also ran a technical ½ day seminar on layout and storage of steam generating plants. This was hugely successful and of value to the NZ water/steam community. Other NZAPWS seminar highlights include more involvement of university researchers.

2. David Addison has had ongoing involvement in the PCC Corrosion Product Sampling working group
3. 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
4. David Addison and Ian Richardson have continued working on geothermal related aspects for a IAPWS white paper along with Nobuo Okita (Toshiba) of Japan
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. He presented a paper ‘Updating the Greenspan “Functional equations” for the water vapour enhancement factor’ at TEMPMEKO 2019 in Chengdu, China.
6. Initial planning has commenced for IAPWS 2021 in New Zealand, likely location will be Rotorua in September 2021 to allow attendees to experience the geothermal wonders of New Zealand.

Publications:

No publications by NZAPWS members in 2018/2019

David Addison
NZAPWS Chairperson
Mobile + 64 21 843 762
Email: david.addison@thermalchemistry.com
Web: www.nzapws.org.nz

Scandinavian IAPWS Committee
c/o IDA, Kalvebod Brygge 31-33
1780 København V

20 September 2019



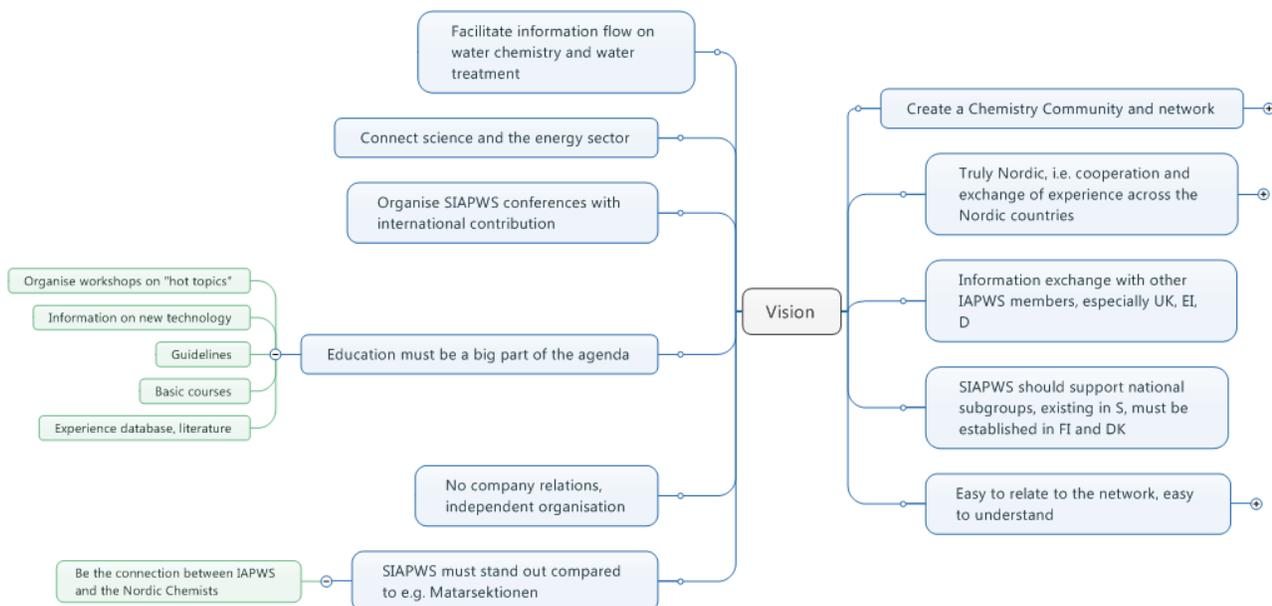
SIAPWS Annual Report for 2018

The discussion at the 2018 SIAPWS annual meeting in March in Södertälje focused on the future of SIAPWS. The general feeling was that even though we had taken many initiatives during the last couple of years, the full impact had yet to come. The exchange of experience in the field between the Nordic countries was still rudimentary, and the poor attendance to the first SIAPWS on-line courses showed that many did not see themselves as a natural part of the network. Thus, there was a need to rethink the role of SIAPWS.

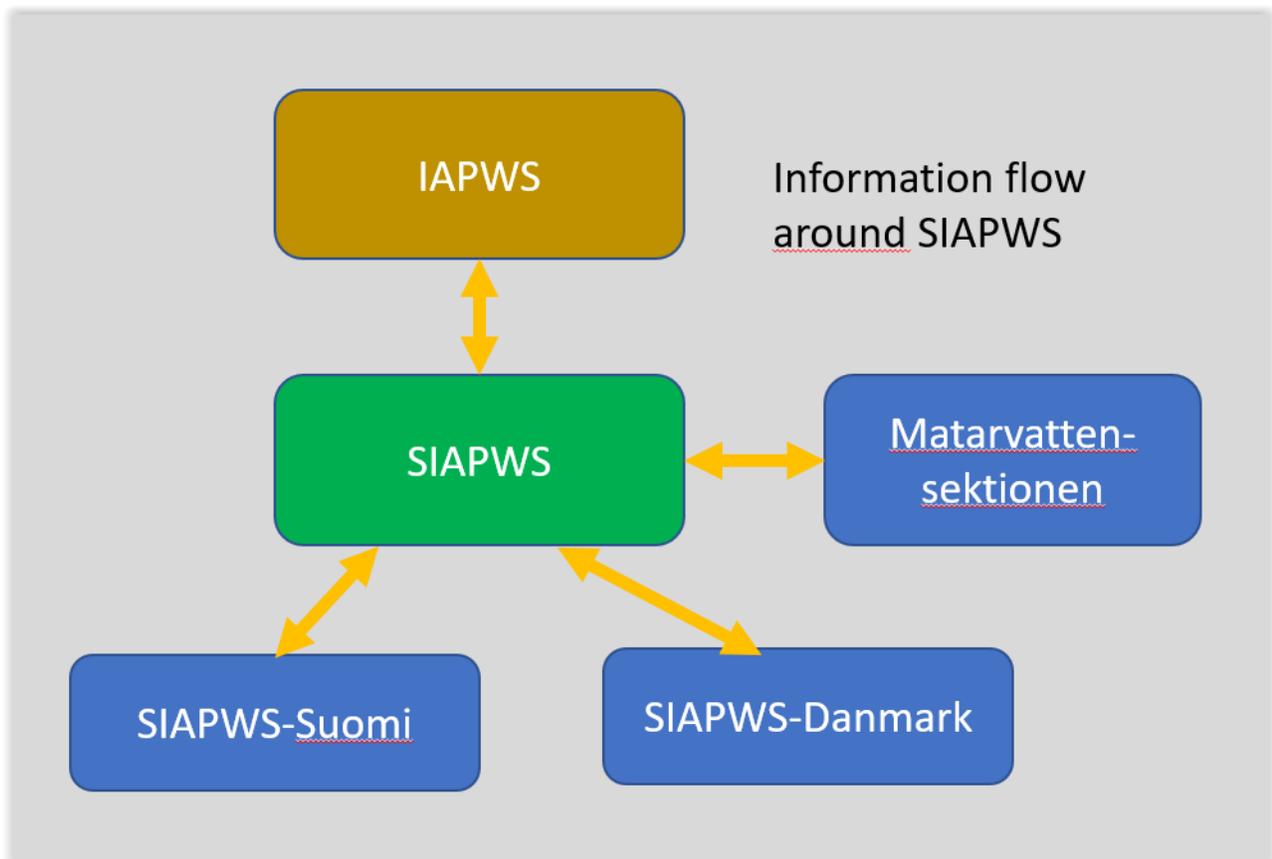
In May 2018 in Helsinki, the newly elected Executive Committee (EC) met for a workshop with this focus and had a couple of productive days with many ideas and discussions. The outcome was a plan transforming SIAPWS to a truly Nordic organisation with national groups in the three countries Sweden, Finland and Denmark. Matarvattensektionen should continue to be the natural representative of the Swedish energy community, whereas SIAPWS would initiate national groups in Finland and Denmark. This recognises that many colleagues feel more comfortable speaking and listening in their own language, but still opens for Nordic and international experience exchange through meetings and communication in English. Easily understandable and efficient communication must be in focus both on national and Nordic level. This setup also calls for organising Nordic conferences with international contribution.

Main purposes of SIAPWS continue to link the Nordic and the international energy chemistry society in IAPWS, to offer education on-line for a modest cost, and to to organise workshops in current topics.

The new vision of SIAPWS is summarised in the mindmap below.



The new mode of operation of SIAPWS is an important change, and the EC will work hard to make a success out of it. The idea is shown in the figure, in which SIAPWS, as usual, relates to the international organization, IAPWS, but also to three national organizations in Sweden, Finland, and Denmark. The two groups in Finland and Denmark are newcomers and have been started in late 2018 and early 2019, whereas Matarvattensektionen takes the national role in Sweden. The national groups will live their own life with an organizing committee, their own meetings and workshops, and members that pay a fee to participate. On top of that, SIAPWS will organize exchange of information and experiences across the national organizations and to and from IAPWS. All members of the national groups are automatically members of SIAPWS also and have access to all information passing through that level. We have so much in common in the Nordic energy industry that it certainly will be of common interest to share experience and knowledge between the groups. The base will be the national groups that make events primarily for their countrymen and in the national language. On top of that everybody is welcome and invited to participate on the Nordic and international level where the language will be English. Those who do so will be the messengers between the national and the international levels. The main objective is to penetrate much more widely into the energy industry and relay valuable information within the Nordic countries and internationally. Both the Finnish and Danish groups have been started up successfully with around 25 companies as registered members. Matarvattensektionen continues to be "big brother" in the organization with a little more than 100 companies as members. These are now direct members of SIAPWS instead of the secondary membership through Matarvattensektionen.



The on-line education evolved in 2018 with 8-15 participants in the later courses on corrosion, preservation, and water-steam chemistry. This means that we have achieved an economical balance where the participant fees pay for the preparation of the courses.

A major highlight in 2018 was the international conference in Prague, ICPWS-17, with a record-high number of participants from the Nordic countries. SIAPWS organized two sessions on the flue gas condensation and re-use of condensate. These turned out successfully with many attendants and large interest for the new green technology that saves fuel costs and water resources while improving the flue gas cleaning at the same time.

Contact Person: Chair Karsten Thomsen
Mail: knth@cowi.dk
Phone: +45 2787 5744

The Swiss National Committee
International Association for the Properties of Water and Steam

Report on IAPWS related activities – September 2018 / September 2019
Submitted to the EC Meeting of IAPWS, Banff, Alberta, Canada – September 2019

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:

- Prof. Dr. Horst-Michael Prasser, Institute of Energy Technology, Swiss Federal Institute of Technology, Zürich, E-Mail: prasser@lke.mavt.ethz.ch
- Dr. Robert Svoboda, Svoboda Consulting, Wettingen, E-Mail: r.l.svoboda@swissonline.ch
- Dr. Michael Hiegemann, General Electric (Switzerland) GmbH, Baden, Switzerland, E-Mail: michael.hiegemann@ge.com
- 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
Vice-chairman of PCC Sub-Task Group on Film Forming Amines (FFA): Marco Lendi
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. The board of SCPWS is currently planning a smaller event in Spring 2020 to find new participating institutions in Switzerland.
- It is therefore requested to extend the Associate Membership for another term.

M. Lendi, September 2019

U.S. National Committee to IAPWS 2019 Report on Activities of Potential Interest to IAPWS

17 September 2019

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

A paper (in conjunction with the Ruhr-University Bochum) describing the new reference equation of state for the thermodynamic properties of heavy water was published:

- *A Reference Equation of State for Heavy Water*, S. Herrig, M. Thol, A. H. Harvey, and E. W. Lemmon; *J. Phys. Chem. Ref. Data* **47**, 043102 (2018) <https://doi.org/10.1063/1.5053993>

In a related 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, and work is underway on a new thermal conductivity correlation.

Analysis was performed on the low-density behavior of IAPWS-95, discovering that 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. A paper is in press in the *International Journal of Thermophysics*.

Work performed last year to describe the second and third virial coefficients of H₂O and D₂O from high-quality intermolecular potentials, in collaboration with researchers at Fondazione Bruno Kessler (Italy), Nicolaus Copernicus University (Poland), and the University of Delaware (USA), has been published:

- *Fully quantum calculation of the second and third virial coefficients of water and its isotopologues from ab initio potentials*, G. Garberoglio, P. Jankowski, K. Szalewicz, and A. H. Harvey; *Faraday Discuss.* **212**, 467-497 (2018) <https://doi.org/10.1039/c8fd00092a>

The History and Heritage Committee of the American Society of Mechanical Engineers (ASME) has approved the nomination of *Standardized Steam Property Tables* as an Historic Mechanical Engineering Landmark. Historic Mechanical Engineering Landmarks are artifacts or systems representing a significant mechanical engineering technology. ASME has designated over 250 landmarks through its History and Heritage Landmarks Program since the program began in 1971; more information can be found at <https://www.asme.org/about-asme/engineering-history/landmarks>. In this case, the designation will be a “virtual” landmark, since no corresponding physical object or site exists. A brochure about the Landmark will be prepared that explains its significance, and once that brochure is completed (sometime in 2020) the Landmark will be officially added on the ASME website.

Communicated from the University of Maryland, College Park

Prof. Mikhail Anisimov notes work on the pattern of property extrema in water's atomistic models and on recent work on thermodynamics of real supercooled water (revisited by including negative pressures and new compressibility data obtained below homogeneous ice nucleation temperatures).

- *Pattern of property extrema in supercooled and stretched water models and a new correlation for predicting the stability limit of the liquid state*, Betul Uralcan, Folarin Latinwo, Pablo G. Debenedetti, and Mikhail A. Anisimov; *J. Chem. Phys.* **150**, 064503 (2019) <https://doi.org/10.1063/1.5078446>

- *Thermodynamics of supercooled and stretched water: Unifying two-structure description and liquid-vapor spinodal*, Frédéric Caupin and Mikhail A. Anisimov; J. Chem. Phys. **151**, 034503 (2019) <https://doi.org/10.1063/1.5100228>

Prof. Jan Sengers reports on Casimir pressures in liquids under shear, noting that Couette flow experiments are commonly done with liquid water. We have found that shear-induced pressure enhancements in such experiments cannot be interpreted in terms of currently available computer simulations. The reason is that in such experiments pressure enhancements due to viscous heating are many orders of magnitude larger than observed in computer simulations that impose isothermal flow conditions.

- *Nonequilibrium Casimir pressures in liquids under shear*, J.M. Ortiz de Zárate, T.R. Kirkpatrick, and J.V. Sengers, Eur. Phys. J. E **42**, 106 (2019) <https://doi.org/10.1140/epje/i2019-11868-9>

Communicated from the ASME Research & Technology Committee on Water and Steam in Thermal Systems

Work on the technical content appears to have been completed and the relevant task group is in the formatting/editing process prior to formal vote for the document on *Consensus on Operating Practices for the Control of Feedwater and Boiler Water Chemistry in Modern Industrial Boilers*.

The ASME deaerator inspection guide is nearing completion in the Committee. This document provides the user with information on how to plan for, conduct, and interpret the results of inspections. The document is aimed at power plant and industrial boiler house staff and aiding those persons in planning for inspections, working with the certified inspector, and understanding the results of the inspection reports.

The committee continues to sponsor sessions at the International Water Conference. In 2019 the conference is in Orlando, Florida, and the committee organized and chairs the following two sessions:

- *Communicating Lessons Learned from Operating Steam Generating Systems*
- *Preventing and Remediating Damage Caused by Chemical Excursions in Industrial Boiler Water*

Communicated from OLI Systems

Aqueous chemistry of rare-earth elements

Under the auspices of the Department of Energy's Critical Materials Institute (CMI), OLI Systems continued to work on the properties of aqueous systems containing rare earth elements in existing and emerging processes associated with diversifying the supply of rare earths and recycling rare earth-containing waste products. Recent work focused on (1) developing a comprehensive model for the behavior of rare earths in sulfate systems and (2) modeling the leaching of rare earths from synthetic phosphogypsum (a high-volume waste containing small concentrations of rare earths) using both mineral acids and biolixiviants. The recent work has been published in the following two papers:

- *Rare earth sulfates in aqueous systems: Thermodynamic modeling of binary and multicomponent systems over wide concentration and temperature ranges*, G. Das, M. M. Lencka, A. Eslamimanesh, P. Wang, A. Anderko, R.E. Riman, and A. Navrotsky; J. Chem. Thermodynamics, **131** 49 (2019) <https://doi.org/10.1016/j.jct.2018.10.020>
- *Bio- and mineral acid leaching of rare earth elements from synthetic phosphogypsum*, P.J. Antonick, Z. Hu, Y. Fujita, D.W. Reed, G. Das, L. Wu, R. Shivaramaiah, P. Kim, A. Eslamimanesh, M.M. Lencka, Y. Jiao, A. Anderko, A. Navrotsky, and R.E. Riman, J. Chem. Thermodynamics, **132** 491 (2019) <https://doi.org/10.1016/j.jct.2018.12.034>

Aqueous chemistry for carbon capture and transportation technologies

OLI Systems continues working on developing simulation methods to help in the optimization of advanced CO₂ capture technologies. In collaboration with SRI International, OLI is working on transformational CO₂ capture process based on a combination of mixed-salt and amine-based working fluids.

In collaboration with the Institute for Energy Technology (Norway), OLI is developing a predictive methodology to evaluate the corrosivity in CO₂ transportation systems. The corrosivity is due to reactions between various impurities, which may, under certain conditions, induce the formation of elemental sulfur and mineral acids (sulfuric and nitric).