IAPWS Canadian National Committee

Annual Report 2018

Submitted to IAPWS EC, Prague, Czech Republic, September 7, 2018

CNC Executive: *William Cook (Chair); Derek Lister; Peter Tremaine; Melonie Myszczyszyn; Rich Pawlowicz; Craig Stuart; Luis Carvahlo; Olga Palazhchenko; Sarita Weeraku, Hugues Arcis*

1. Canadian National Committee: Dues for the Canadian National Committee (CNC) of IAPWS are supported by the National Research Council (NRC) of Canada. This arrangement requires support and participation by a national organization representing industry. We are currently in the third year of an agreement with the CANDU Owners Group (COG) and the NRC for a third five-year term.

The CNC recruited Luis Carvalho, Olga Palazhchenko, Sarita Weerakul, Hugues Arcis to the committee to help with preparations to host the 2019 IAPWS Annual Meeting to be held in Banff, Canada.

2. CNC Activities

2.1 CNC Workshop 2017

The CNC hosted an IAPWS workshop on December 13, 2017 at the offices of COG in the heart of downtown Toronto that attracted 33 participants. The workshop, web-cast across Canada and with invited presenters from the USA, included presentations from all working groups and showed the breadth of IAPWS's work and its relevance. The goal was to raise the profile of the Canadian National Committee and IAPWS activities with scientists and engineers in Canada doing complementary research within the fossil and HRSG community. The list of presentations is included at the end of this report.

2.2 Activities at the University of New Brunswick (UNB)

Derek Lister

Under the title of UNB Nuclear, the Research Chair in Nuclear Engineering at UNB continues with traditional funding from the CANDU Owners Group and the Natural Sciences and Engineering Research Council, supplemented with contracts from the Electric Power Research Institute and companies such as Kurita Japan.

Heat exchanger fouling; the damaged atmospheric-pressure water loop has been repaired and a program for studying magnetite particle transport with additions of film-forming amines (FFAs) is being initiated. Bench studies of adsorption of film-forming amines on magnetite, with experiments on magnetite powder and sintered magnetite pellets, have provided preliminary data on the adsorption kinetics.

Flow-accelerated corrosion (FAC); experiments on the effects of an FFA on FAC in a recirculating water loop are underway. Under two-phase steam-water conditions at 200°C, the durability of FFA films adsorbed on carbon steel is being tested by exposing them to different shear-stress conditions by varying the average velocities of the fluid. Other FAC-related studies are providing data on the magnetite dissolution rate constant under conditions of reducing chemistry in feedwater systems and are developing a neural network scheme for predicting FAC rates by learning from the wealth of experimental data collected at UNB Nuclear over the years.

Modelling reactor primary circuit contamination; in collaboration with UNB's Centre for Nuclear Energy Research (CNER), progress has been made in developing a comprehensive model for activity transport in the Point Lepreau primary coolant. In parallel, studies in a high-temperature water loop under CANDU primary coolant conditions have provided preliminary values of the magnetite precipitation constant, to be reinforced later with values from radiotracer experiments.

Measuring the effusion rate of hydrogen through steel; in a collaborative project with CNER, the development of an in-situ probe (HEPro) for monitoring FAC by measuring the rate of effusion of corrosion hydrogen through pipe walls is being supported by investigating with computational fluid dynamics the details of hydrogen diffusion around the probe structure. At the same time, experiments have measured rates of effusion of hydrogen through carbon steel piping under various conditions and the results are being modelled.

Investigating the corrosion of aluminium alloy under the conditions of reactor coolant released during a severe loss-of-coolant accident; during a LOCA, corrosion products released from aluminium components in containment can block the sump strainers and impede access of the emergency core cooling system (ECCS) to the reactor fuel. The rates of release of Al species to typical reactor coolant have been measured under a range of possible LOCA conditions and the dependence on chemistry and flow rate determined. In parallel, the corrosion of 3-D printed components is compared with that of the standard cast alloy.

Willy Cook

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

CNER has recently partnered with the provincial government and several advanced nuclear reactor designers and vendors with the intention of establishing a Small Modular Reactor Research Cluster within the Province.

CNER's HEPro has continued to demonstrate its utility and sensitivity for measuring changes in FAC rate of carbon steel. Several COG programs are now in progress and additional installation of HEPro for feeder pipe and feed water pipe monitoring are being planned for 2019.

W. Cook and D. Addison (Thermal Chemistry Inc. – New Zealand) have completed the first phase of an IAPWS International Collaboration project that was initiated in 2015. The focus of the project was to establish capabilities at UNB / CNER's laboratories to measure, electrochemically, the effects of mixed contaminants on boiler materials. D. Addison again visited UNB / CNER in June 2018 to carry out some of the experimental testing.

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

The NSERC/UNENE Senior Industrial Research Chair in High Temperature Aqueous Chemistry was awarded to Professor Peter Tremaine at the University of Guelph in 2016. The purpose of the Chair is to expand mission-oriented basic research and modelling expertise in areas related to the primary coolant chemistry, moderator chemistry, and steam-generator chemistry of the CANDU reactor fleet, as well as in areas related to the geological storage of nuclear spent fuel. The funding model is new for a UNENE IRC, in that support has been provided by three other industrial partners, in addition to UNENE: the CANDU Owner's Group (COG), the Nuclear Waste Management Organization (NWMO) and the Electric Power

Research Institute (EPRI). Additional support from NSERC and the University of Guelph is also being provided, including the recruiting a tenure-track assistant/associate professor in an area of research related to the IRC activities.

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

IAPWS-related activities continue to concentrate on investigations into the effect of chemical composition changes in seawater on its physical properties, and coordination of international activities in supporting and extending the seawater standard TEOS-10 through chairmanship of the Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS).

2.5. CANDU Owner's Group (COG) Activities

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

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

COG is the primary sponsor for the CNC to host the 2019 IAPWS Annual Meeting. Financial support has be received to secure our booking at the Banff Centre for the Arts and Creativity and COG's willingness to back the CNC to secure this venue is much appreciated.

2.6 Oil Industry Activities (Melonie Myszczyszyn, Canadian Natural Resources Ltd.)

M. Myszczyszyn is participating in multiple industry driven water initiatives with the goal to resolve oil and gas related water scaling and corrosion mechanisms.

Initiative # 1) WTDC (water treatment development centre) is being built up at the Suncor Firebag facility in Fort McMurray and will operate from 2018 to 2024 onwards. This test facility will be used to live feed stream test produced water with various water treatment technologies to find better ways to soften, de-oil, heat exchange, and make steam for oil and gas operations. Goal to advance the technologies used to treat produced water and make steam for thermal injection oil recovery method. Melonie is the WTDC Mancomm project manager for CNRL shares in the WTDC.

Initiative #2) Other spinoffs from the WTDC larger facility trial system is the development of the NAIT and SAIT and U of C laboratory testing trial facilities being created for doing smaller sized water to steam generation scale and corrosion investigations. These spinoff lab testing projects are being done by COSIA water and championed by Suncor oil and gas company and other oil and gas operators. Melonie is providing her OTSG (once through steam generator) knowledge in the design of these lab testing smaller OTSG version test trials.

Initiative #3) CRIN water theme – Melonie is the CNRL representative in this theme – CRIN water theme is a Canadian initiative to link all water related entities, create water connectivity roadmaps to show water entrepreneurs all the water links that exist and connect them to the research/academic communities like

IAPWS for water and governmental funding opportunities W. Cook attended the recent CRIN water theme meeting and will participate on behalf of IAPWS and share IAPWS capabilities with the other water entities.

Initiative #4) linking COSIA in-situ and mining entity with IAPWs by extending the invitation for the 2019 IAPWS Banff Conference to the industry operators that attend COSIA. Shared information about IAPWS with COSIA water contacts John Brogly and Chris Godwaldt. The hope is that the oil and gas industry operators within Alberta will be able to attend this 2019 IAPWS conference in Banff as is located close to Calgary, Alberta.

In November (28-29), at the 6th Water Management Initiative Canada 2018, Melonie is scheduled to give a presentation on "advancements in technologies and new initiatives for treating produced water for recycling & reuse".

4. Activities Planned

The CNC activities over the next few years will continue the work that is currently ongoing, as described above.

The CNC is now in the full planning stages for hosting the 2019 IAPWS meetings. The venue and dates have been finalized and the meeting will take place at the Banff Centre for Arts and Creativity between Sunday September 29 – Friday October 4, 2019.

5. Select List of Publications

1. Applegarth, L., Pye, C., Cox, J. S., & Tremaine, P. R. (2017). A Raman Spectroscopic and Ab Initio Investigation of Aqueous Boric Acid, Borate and Polyborate Speciation from 25 to 80 °C. *Industrial & Engineering Chemistry Research, 56*, 13983-13996, doi: 10.1021/acs.iecr.7b03316.
2. McGregor, C., Fandino, O., Cox, J. S., Ballerat-Busserolles, K., & Tremaine, P. R. (2017). Standard Partial Molar Heat Capacities and Volumes of Aqueous N-Methylpiperidine and N-Methylpiperidinium Chloride from 283 K to 393 K. Journal of Chemical Thermodynamics, 113, 377-387, doi: 10.1016/j.jct.2017.05.033.
3. Ferguson, J. P., Arcis, H., Zimmerman, G. H., & Tremaine, P. R. (2017). Ion-Pair Formation Constants of Lithium Borate and Lithium Hydroxide under Pressurized Water Nuclear Reactor Coolant Conditions. Journal of Chemical Thermodynamics, 56, 8121-8132, doi: 10.1021/acs.iecr.7b01015.
4. Nieto Roca, D. E., Romero, C. M., & Tremaine, P. R. (2017). Ionization constants of DL-2-aminobutyric acid and DL-norvaline under hydrothermal conditions by UV-visible spectroscopy. Journal of Solution Chemistry, 46, 388-423, doi: 10.1007/s10953-017-0569-z.
5. Lowe, A. R., Cox, J. S., & Tremaine, P. R. (2017). Thermodynamics of Aqueous Adenine: Standard Partial Molar Volumes and Heat Capacities Of Adenine, Adeninium Chloride and Sodium Adeninate from T = 283.15 K to 363.15 K. Journal of Chemical Thermodynamics, 112, 129-145, doi: 10.1016/j.jct.2017.04.005.

6. Arcis, H., Ferguson, J. P., Applegarth, L. M., Zimmerman, G. H., & Tremaine, P. R. (2017). Ionization of Boric Acid in Water from 298 K to 623 K by AC Conductivity and Raman Spectroscopy. Journal of Chemical Thermodynamics, 106, 187-198, doi: 10.1016/j.jct.2016.11.007.
7. Alcorn, C., Cox, J., Applegarth, L., & Tremaine, P. R. (2017). Quantitative Raman Investigation of Uranyl Sulfate Complexation under Hydrothermal Conditions. *Proc. 37rd CNS Student Conf.*
8. Ferguson, J., Arcis, H., Hussey, D., Wells, D., & Tremaine, P. R. (2017). Boric Acid Ionization Constants and Triborate Formation Constants under PWR Primary Coolant Conditions by AC Conductivity. *Proc. 37rd CNS Student Conf.*
9. Palazhchenko, O.Y., Cook, W.G and Taylor, D., *UNB CANDU-6 Primary Heat Transport System Code: Development and Validation of a Thermal-Hydraulic Expansion,* Accepted to the 2018 Canadian Nuclear Society Annual Conference, Saskatoon, SK, June 2018.
10. Steeves, G. and Cook, W.G., *Development of Kinetic Models for the Long-term Corrosion Behaviour of Candidate Alloys for the Canadian SCWR,* Journal of Nuclear Engineering and Radiation Science, vol.3, no.3, pp. 031001-031000-7, July 2017.

IAPWS - CANADIAN NATIONAL COMMITTEE WORKSHOP
(CNC-IAPWS)

December 13, 2017
Korea Room, COG Office
17th Floor, 655 Bay Street, Toronto, ON

FINAL AGENDA

	1.0	Introduction to IAPWS	
8:30 – 8:40	1.1	Welcome and Introduction	Willy Cook (UNB)
8:40 – 9:00	1.2	Background on IAPWS and the CNC-IAPWS	Willy Cook (UNB)
9:00 – 9:30	1.3	Current IAPWS Activities	Barry Dooley (Structural Integrity)
9:30 – 10:00	1.4	Candu Owners Group (COG) – IAPWS synergies between the nuclear and fossil industries	Steve McGee (COG)
10:00 – 10:15	Coffee break		
	2.0	Cycle Chemistry and Use of Film Forming Amines and Film Forming Products	
10:15 – 10:45	2.1	Optimum Cycle Chemistry for Fossil and Combined Cycle Plants	Barry Dooley (Structural Integrity)
10:45 – 11:15	2.2	COG FFA Programs	John Krasznai (COG)
11:15 – 11:45	2.3	Adsorption of FFPs and Effects on FAC (some of the studies at UNB Nuclear)	Derek Lister (UNB)
11:45 – 12:15	2.4	FFA use in Water Systems in the Oil & Gas Industry	Ivan Morales (Devon Canada)
12:15 – 12:45	2.5	IAPWS White Paper on FFA/FFP use in Nuclear Plants	Willy Cook (UNB)
12:45 – 1:30	Lunch		
	3.0	Modelling of Aqueous Systems in Harsh Environments	
1:30 – 2:00	3.1	Introduction to OLI Models and Case Studies	Andre Anderko (OLI)
2:00 – 2:30	3.2	Introduction to MultEQ and Uses	Dan Wells (EPRI)
2:30 – 3:00	3.3	Modelling Seawater Properties and their Implications for Industrial Systems	Rich Pawlowicz (UBC)
3:00 – 3.30	3.4	Case Studies of Modelling in Oil & Gas Processing	Subodh Peramanu (CNRL)
3:30 – 3:45	Coffee break		
	4.0	Emerging Issues & Technologies for the Use of Water and Steam	
3:45 – 4:15	4.1	High Temperature Reverse Osmosis Membranes	Basil Perdicakis (Suncor)
4:15 – 4:30	4.2	Generation Capacity and Trends in Ontario	Brian Townes (OPG-Lennox)
4:30 – 4:50	4.3	Group Discussion on Future Technologies / Activities	all
	5.0	Closing Discussion	
4:50 – 5:00	5.1	New CNC-IAPWS initiatives and membership	all
5:00	5.2	Workshop wrap-up	Willy Cook
5:30	5.3	Dinner at local establishment	

Czech Society for the Properties of Water and Steam

2018 Annual Report

Submitted to IAPWS Executive Committee in Prague, Czech Republic, September 2018

Because of a change of legislation, the Czech National Committee for the Properties of Water and Steam (CZNCPWS) was replaced by the Czech Society for the Properties of Water and Steam (CZPWS) by the end of 2017. On the contrary to CZNCPWS, which has been one of numerous committees embedded in the structure of the Czech Academy of Sciences, CZPWS is a standalone legal entity (Registered Association). All active members of the former CZNCPWS became CZPWS members. The seat of CZPWS is again the Institute of Thermomechanics of the Academy of Sciences of the Czech Republic (IT CAS) in Prague.

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
CZPWS was established at a constituent meeting on October 27, 2017, at IT CAS. Here, the CZPWS Statutes have been adopted. Consequently, the legal status of a Registered Association has been approved on December 4, 2017.
The first annual meeting of the CZPWS was held on June 20, 2018. Strategies to ensure CZPWS funding have been adopted. Activities of IAPWS WGs have been discussed. A significant activity was organizing the 17th ICPWS in Prague.

RESEARCH ACTIVITIES
Surface tension of supercooled water was studied at IT CAS in Prague and at the University of West Bohemia (UWB) in Pilsen.

Measurements of pure water under supercooled conditions conducted at IT CAS were finalized [1]. The measurements with the horizontal capillary tube imitating original method employed by P.T. Hacker [NACA TN 2510 (1951)] did not confirm the second inflection point anomaly down to -23 °C. The new data are in good agreement with the previous measurements conducted with the capillary rise technique employed in the extrapolation of the IAPWS standard [Hrubý et al., J. Phys. Chem. Lett. 5 (2014) 425 and Vinš et al., J. Phys. Chem. B 119 (2015) 5567]. The experimental apparatus has been further modified and is being used for the measurements of supercooled aqueous mixtures. Preliminary data for the surface tension of binary mixtures of water with methanol, ethanol, and propanol were presented at the international conference EFM 2017 [6]. Currently, the new measurements with supercooled seawater are carried out in order to verify extrapolation of the seawater correlation by Nayar et al. [J. Phys. Chem. Ref. Data 43 (2014)] in the supercooled region. For the needs of the task group, V. Vinš wrote an internal report “Surface tension of seawater at low temperatures including supercooled region down to –25 °C”.

At UWB, R. Mareš continued in surface tension measurements in the supercooled region down to -32°C (mentioned in Kyoto 2017). J. Kalová and R. Mareš tested a new equation for the surface tension of water

(results will be presented in Prague, ICPWS17th in Prague). J. Kalová and R. Mareš also published a work on the mean field equation of state for supercooled water [7].

At IT CAS, additional measurements for the density of supercooled water have been performed and a new data set on the density of supercooled seawater has been recorded [8].

In an international collaboration of the Ruhr-Universität Bochum, the Technische Universität Dresden and IT CAS, a thermodynamic model for eight pure gas hydrates relevant mostly for CCS (Carbon Capture and Storage) applications was successfully extended to hydrate mixtures. The complex phase equilibrium algorithms developed for various fluid phases, gas hydrates, and pure solid phases (ices) were thoroughly revised in order to model multicomponent systems with mixed hydrates. The results were published in Fluid Phase Equilibria [5] and presented at a German national conference [9].

Researchers from IT CAS (J. Hrubý, M. Duška, T. Němec) and M. Kolovratník from the Czech Technical University in Prague published a study on nucleation in steam and water vapor – carrier gas mixtures, including data from steam nozzles, turbines, classical nucleation data, and molecular simulations, including own simulations with TIP4P/2005 force field [2]. A team from the Institute of Chemical Process Fundamentals and IT CAS finalized a study of nucleation in mixtures of sulfuric acid and water vapors using a new experimental method [3].

At SIGMA Research and Development Institute and the Centre of Hydraulic Research, M. Sedlář and coworkers were developing models of cavitation erosion during the hydrodynamic cavitation and models of cavitation instabilities in hydrodynamic pumps [10]. In cooperation with ITCAS, 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. 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].

At Doosan Škoda Power, P. Rudasová was concerned with the implementation of IAPWS guidelines for operating blocks. The implementation of IAPWS Technical Guidance Documents in Czech power plants is difficult, most personnel adhere to outdated national technical standards.

Publications

1. Vinš V., Hošek J., Hykl J., Hrubý J.: *Surface tension of supercooled water: Inflection point-free course down to 250 K confirmed using a horizontal capillary tube*, J Chem Eng Data 62 (2017) 3823-3832.
2. Hrubý J., Duška M., Němec T., Kolovratník T.: *Nucleation rates of droplets in supersaturated steam and water vapour–carrier gas mixtures between 200 and 450K.* J Power and Energy 232 (2018) 536–549.
3. Trávníčková T., Škrabalová L., Havlica J., Krejčí P, Hrubý J., Ždímal V. *Laboratory study of H2SO4/H2O nucleation using a new technique – a laminar co-flow tube*, Tellus B Chem Phys Meteorol 70 (2018) 1446643.
4. Sedlar, M., Soukal, J., Komarek, M., Volkov, A.V. and Ryzhenkov, A.V.: *Numerical Simulation of Interaction between Fluid and Vapor Structures in Multiphase Flow around Hydrofoil*. Journal of Applied Mathematics and Physics, 2018, under review
5. Hielscher S., Vinš V., Jäger A., Hrubý J. Breitkopf C., Span R.: *A new approach to model mixed hydrates*, Fluid Phase Equilibria 459 (2018) 170-185.

Conference Presentations

6. Vinš V., Hykl J., Nikl Z., Čenský M., Hrubý J.: *Surface tension of aqueous binary mixtures under the supercooled conditions – Development of the measuring technique and preliminary data for water + lower alcohols*, international conference Experimental Fluid Mechanics 2017, Mikulov (Czech Rep.), November 21-24, 2017.

7. Kalová J., Mareš R.: *Mean-Field Equation of State of Supercooled Water and Vapor Pressure Approximations,* AIP Conference Proceedings 1889, 020016 (2017)

8. A. Blahut, M. Duška, J. Hykl, P. Peukert, V. Vinš, M. Čenský, J. Hrubý, *Dual-Capillary Apparatus for Accurate Density Measurements of Supercooled Water*, Twentieth Symposium on Thermophysical Properties, Boulder (CO, USA), June 24-29, 2018.

9. Hielscher S., Jäger A., Vinš V., Breitkopf C., Hrubý J., Span R.: *Modellierung gemischter Gashydrate konsistent zu vielparametrigen Zustandsgleichungen*, Thermodynamik Kolloquium 2017, Dresden (Germany), September 27-29, 2017.

10. Sedlář, M.: *Cavitation phenomena in balancing drums of high-performance feed pumps.* PCC/PCAS/IRS Joint WG Meeting and Workshop, IAPWS Meeting, Kyoto, 2017.

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 2017/2018

www.iapws.de

Chair: Ingo Weber, Siemens Power and Gas, Erlangen

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

Annual Meeting of the German National Committee

The 2018 Annual Meeting of the German National Committee took place at the Leibniz Institute for Tropospheric Research in Leipzig on 9th March 2018. 23 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.:
  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.
  Volume 165, July–August 2018, Pages 268-286 (2018).
  https://doi.org/10.1016/j.pocean.2018.04.004, in press
- 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
- Hellmuth, O.; Shchekin, A.K.; Feistel, R.; Schmelzer, J.W.P.; Abyzov, A.S.:
  Physical Interpretation of Ice Contact Angels, Fitted to Experimental Data on Immersion Freezing of Kaolinite Particles.
  Interfacial Phenomena and Heat Transfer, 2017 (in press).
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.
  N.N. (2018), in preparation.
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air".
  N.N. (2018), in preparation.

Baltic Sea Research Institute, Warnemuende
Dr. Stefan Weinreben

Projects

1. Measurements of density and practical salinity in the Baltic Sea to determine the absolute salinity anomaly
2. Preparation of a paper about measurements of the density-anomaly in the Atlantic Ocean.
3. We got the ILAC-accreditation for the calibration laboratory of the IOW for the calibration of oceanographic devices for electrical conductivity, temperature and pressure.

German Aerospace Center (DLR), Cologne
Institute of Propulsion Technology
Prof. Dr. Francesca di Mare

Project

1. Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the CFD Code TRACE.
   - 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 CFD code TRACE.
   - On this basis the implementation has been further improved, especially regarding the software architecture, solution algorithm and boundary treatment.
   - The capability of the SBTL-method has been tested on Laval-nozzle and Cascade test cases. The calculation of a real steam engine configuration is targeted next.

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.

Leibniz Institute for Tropospheric Research, Leipzig
Dr. Olaf Hellmuth

Projects

1. Preparation of a Paper about Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air
2. Preparation of Three Further Volumes on New Particle Formation in the Earth Atmosphere

Recent Publications

- Hellmuth, O.; Shchekin, A.K.; Feistel, R.; Schmelzer, J.W.P.; Abyzov, A.S.:
  Physical Interpretation of Ice Contact Angels, Fitted to Experimental Data on Immersion Freezing of Kaolinite Particles.
  Interfacial Phenomena and Heat Transfer, 2017 (in press).

- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.
  N.N. (2018), in preparation.
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air".
  N.N. (2018), in preparation.

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

Projects:

1. Development of a new reference equation of state for heavy water. This work is linked to an IAPWS grant awarded in 2012 and to a close cooperation with Dr. A. H. Harvey and Dr. E. W. Lemmon at NIST in Boulder, CO. The work on the new equation of state has largely been finished. A draft release will be submitted to the evaluation task group and were presented at the 2017 IAPWS meeting in Kyoto.
2. The work on a new mixed gas hydrate model consistent to reference equations of state 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 pure hydrate formers was recently successfully modified in order to allow the calculation of mixed gas hydrates, which resulted in a publication by Hielscher et al. (2018) and another planned publication for this year.

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 (2018), submitted.
- Hielscher, S.; Vinš, V.; Jäger, A.; Hrubý, J.; Breitkopf, C.; Span, R.:
  A New Approach to Model Mixed Hydrates,
  Fluid Phase Equilib. 459 (2018), 170–185.

Ruhr University Bochum
Faculty of Mechanical Engineering, Chair of Thermodynamics
Prof. em. Dr. Dr. e. h. Wolfgang Wagner

Project

1. Preparation of the 3rd edition of the book "International Steam Tables".

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.

Siemens Energy Solutions, Erlangen
Michael Rziha

Projects

1. Development of new Technical Guidance Documents:
   - Air In-Leakage in Steam Water Cycles. Finally developed, so that the release can be expected in 2018
   - Ensuring the Integrity and Reliability of Demineralized Makeup Water Supply to the Unit Cycle. TGD is drafted, but still some work needs to be done. Release is expected by 2019
   - Film Forming Products. Following the release of the IAPWS TGD on FFP for Fossil and Combined Cycle Plants and the IAPWS International Conference on FFP in Lucerne and a 2nd conference in Prague in spring 2018, IAPWS will be developing two new TGD on FFP:
     a) Application of Film Forming Products in Nuclear Plants.
     b) Application of Film Forming Products in Industrial Plants.
   - Both TGD's are progressing, however still some work to be done, so release is not expected before 2019.
2. Developing of white papers as basis for future technical guidance documents
   - Monitoring Corrosion Products in Flexible (cycling and two-shifting) Plants. White paper is developed for presentation at the 2017 Meeting. TGD will be further developed based on this input.
   - Aspects of Geothermal Steam Chemistry. A White Paper for the 2017 Meeting is in preparation. This will be used to determine if a TGD can be developed.

Highlight:

- IEC has finally agreed to withdraw their standard IEC 61370 Ed 1.0: 2002 Steam turbines - Steam purity in favor of IAPWS TGD5-13, due to the fact that the IAPWS TGD on steam purity is the most modern, state of the art and international accepted guidance on this topic. This is underlining once more the huge international leadership of IAPWS on aspects of high-temperature steam, water and aqueous mixtures relevant to thermal power cycles.
- A so called category C liaison (which is some sort of loose liaison, just for exchange of information) between IEC - MT12 and IAPWS PCC Working Group will be established.

Siemens Energy Solutions, Erlangen
Ingo Weber, Stefan Bennoit, Julien Bonifay

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, Faculty of Mechanical Science and Engineering, Thermodynamics
Prof. Dr. Cornelia Breitkopf
Dr. Andreas Jäger, Dr. Tommy Lorenz, Erik Mickoleit

Projects:

1. The work on a new mixed gas hydrate model consistent to reference equations of state 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 pure hydrate formers was recently successfully modified in order to allow the calculation of mixed gas hydrates, which resulted in a publication by Hielscher et al. (2018) and another planned publication for this year.
2. 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).
3. A new predictive mixing rule for the multi-fluid mixture model was developed and published (Jäger et al. (2018)). The new mixture model involves a theoretically based departure function, which allows for the combination of the multi-fluid mixture model with excess Gibbs energy models, like UNIFAC or COSMO-SAC. The application of this new model to mixtures containing water is ongoing work (Dr. Andreas Jäger, Erik Mickoleit). Results of the new model will be presented on the 17th ICPWS in Prague (2018).

Recent Publications

- Hielscher, S.; Vinš, V.; Jäger, A.; Hrubý, J.; Breitkopf, C.; Span, R.:
  A New Approach to Model Mixed Hydrates.
  Fluid Phase Equilib. 459, 170–185 (2018).
- Jäger, A.; Bell, I.H.; Breitkopf, C.:
  A theoretically based departure function for multi-fluid mixture models, Fluid Phase Equilib. 469, 56–69 (2018).

University of Rostock, Rostock
Institute of Chemistry, Department of Physical Chemistry
Dr. Robert Hellmann

Project

1. *Ab-initio* Calculations for Transport Properties of Water and Aqueous Mixtures.

Recent Publications

- Hellmann, R.:
  Cross Second Virial Coefficient and Dilute Gas Transport Properties of the (H2O+CO2) System from First-Principals Calculations,
  Fluid Phase Equilib. (2018), submitted.

VGB PowerTech e.V., Essen
Dr. Andreas Wecker

Project

1. *Development of a new VGB- standard*: Chemical Feeding and Feed Systems for Water/Steam Circuits.
   - This VGB-Standard supplements the VGB Standards for "Feed Water, Boiler Water and Steam Quality for Power Plants / Industrial Plants" and VGB-Standard "Sampling and Physico-Chemical Monitoring of Water and Steam Cycles" and contains recommendations for the correct location, design and instrumentation as well as operation and maintenance of chemical feed equipment in the water/steam circuit. It was published in July 2018.
   -

Zittau/Görlitz University of Applied Sciences
Department of Technical Thermodynamics
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
   - Non-stationary thermo-hydraulic codes SubChanFlow and TwoPorFlow of the Karlsruhe Institute of Technology KIT
   - Non-stationary thermo-hydraulic code RELAP-7 of the Idaho National Laboratory INL
   - Heat-cycle simulation program EBSILON of STEAG Energy Services
   - Heat-cycle simulation program KRAWAL of Siemens Energy Solutions
   - Non-stationary heat-cycle simulation program DYNAPLANT of Siemens Energy Solutions.

3. Development of algorithms for the transport properties of moist air, ASHRAE Research Project 1767.
4. Preparation of a new ASHRAE standard for calculating moist air properties, ASHRAE Project SPC 213P.
5. Reworking on the 3rd edition of the book "International Steam Tables".

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.
- Kunick, M.:
  Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL).
  Fortschritt-Berichte VDI, Reihe 6 Energietechnik, Nr. 618 (2018).
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.
  N.N. (2018), in preparation.
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air".
  N.N. (2018), in preparation.

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS, Prague, Czech Republic, September 2018

Japanese National Committee, Chaired by Professor Masaru Nakahara
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)
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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. We have the successfully organized IAPWS Annual Meetings in the last summer, 2017 and reported the international cooperation achievements; see 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 about 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
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[1] Nakahara, M.; Yoshida K.; “Handbook of Scientific Tables”, Maruzen Publishing Co., Ltd., Tokyo and World Scientific Publishing Co, Singapore, in press.

Hirano, Hideo
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Yasuoka, Kenji
Professor, Department of Mechanical Engineering, Keio University
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Parameters for 1-Parmitoyl-2-Oleoyl Phosphatidyl Choline (POPC) Membrane", Chem. Phys. Lett., 684, 427-432 (2017). DOI: 10.1016/j.cplett.2017.07.032
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[3] Doi, H.; Yasuoka, K.; "Replica Exchange Molecular Simulation of Lennard -Jones Particles in a Two-Dimensional Confined System", AIP Advances, 7, 055018 (9 pages) (2017). DOI: 10.1063/1.4984815
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New Zealand Association for the Properties of Water and Steam (NZAPWS) Annual Report

Date: 27 August 2018

Key Achievements:

1. NZAPWS is now into its second year of full IAPWS membership

2. NZAPWS has robust funding in place and has gained additional sponsors for the 2018/2019 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

Key Activities:

1. A very successful technical seminar was held in May 2018 in Rotorua, NZ with 60 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

This seminar was expanded out to a 2 day program based on NZAPWS member demands and included a NZAPWS networking dinner.

Bobby Svoboda and Derek Lister attended as invited IAPWS members both presenting on their IAPWS related work and areas of interest and Bobby presented a ½ day steam turbine deposits and corrosion technical seminar. This was hugely successful.

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

5. Jeremy Lovell-Smith has continued to contributed to (a) TPWS through continuing investigation into the use of Generalised Least Squares (GLS) to propagate input data covariance into the IAPWS equation parameters and to (b) JCS through work on the definition of relative humidity.

Publications:

1. *P.A Siratovich , M.C. Villeneuve, S. Mordenskym I. Richardson, Acid Solubility Testing of Greywacke Core and Implications for Well Permeability Enhancement, New Zealand Geothermal Workshop, 2017*

2. *T. A. Clark and I. M. Richardson, Hydrogen Peroxide as a Geothermal Cooling Water Biocide, New Zealand Geothermal Workshop, 2017*

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1 September 2018

SIAPWS annual report for 2017

The annual meeting 2017 took place at Brista CHP north of Stockholm and was successful with around 20 participants, good discussion and interesting presentations. It was interesting to learn about Brista's steps towards a flue gas condensate rinsing process that could actually fulfil the demanding environmental limits and to visit the plant afterwards. The discussion focused on the continued introduction of the SIAPWS Water Chemistry Network.

This network has been the focus point of many EC meetings during the year. We have tried to promote it best possible, but with somewhat limited success. The first on-line courses on the interconnection between corrosion and water chemistry was held in late spring and repeated in September. On both occasions, a handful participants took part and there was room for more. The evaluation of the course was good, so we believe that the content and the form of it was OK.

The SIAPWS delegation at the IAPWS annual meeting in 2017 in Kyoto, Japan, consisted of three persons. It was an interesting week both from the cultural and technical viewpoint. The Japanese hosts did a splendid job and proved great hospitality. The Power Cycle Chemistry (PCC) workshops were focused on the Technical Guidance Documents (TGDs), but some presentations were of more general interest.

In the fall, the SIAPW Chair (Karsten) was on a promotion tour in Finland to tell about the work in SIAPWS and IAPWS and invite the Finnish colleagues to become a part of this cooperation. The occasion was a meeting in the Finnish VGB Chemistry Group, and the members present were positive towards SIAPWS.

At the Matarvattenkonferensen in November in Stockholm, SIAWS gave two presentations, one informing about the activities and the other of more general character.

The membership has increased with 5 companies in 2017, and at least 6 will join 2018 leading to nearly 30 in total.

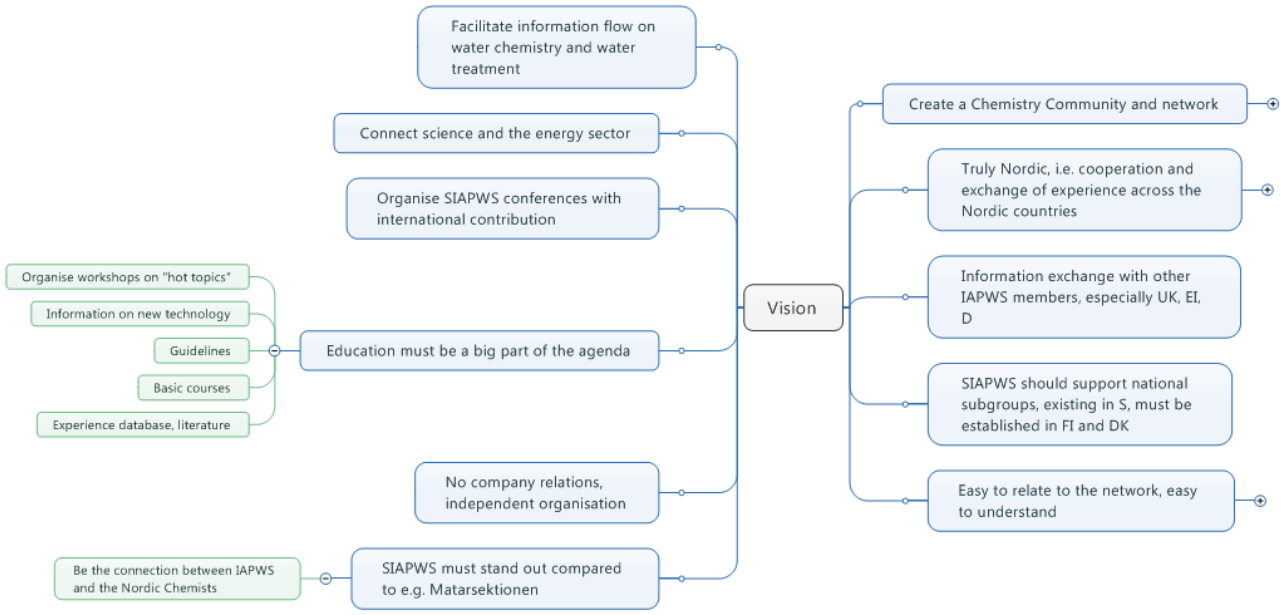
In the spring of 2018, SIAPWS has organised two on-line courses in component failures / plant inspection and plant preservation. We had 10-15 participants on both occasions and again enjoyed good critic afterwards, so this was very satisfactory.

The annual meeting 2018 was hosted by Igelstaverket in Södertälje. We had around 20 participants again, and it was interesting to learn about the very precise fuel (wood chips from forest and waste wood) management at the plant. This is due to rather limited space for fuel storage. The discussion at this SIAPWS annual meeting 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 has yet to come. The exchange of experience within the field between the Nordic countries is still rudimentary, and the somewhat low attendance to the first SIAPWS on-line courses shows that many do not see themselves as a natural part of the network. Thus, there is a need to rethink the role of SIAPWS.

In May in Helsinki, the newly elected Executive Committee (EC) met for a workshop with that focus and had a couple of productive days with many ideas and discussions. The outcome is a plan transforming SIAPWS to a truly Nordic organisation with national groups in the three countries Sweden, Finland and Denmark.

Matarvattensektionen continues to be the natural representative of the Swedish energy chemists, whereas SIAPWS will 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 also calls for organising Nordic conferences with international contribution.

Main purposes of SIAPWS continue to be the link between the Nordic and the international energy chemistry society in IAPWS, to offer education on-line for a modest cost, and to organise work¬shops for current topics. The new vision of SIAPWS is summarised in the mindmap below.



Executive Committee

Chair	Karsten Thomsen	Secretary/cashier	Monika Nielsen
Vice-chair, coordinator	Roger Lundberg	Member	Arja Lehikoinen

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The Swiss National Committee

International Association for the Properties of Water and Steam

Report on IAPWS related activities – September 2017 / August 2018

Submitted to the EC Meeting of IAPWS, Prague, Czech Republic – September 2018.

National Committee Contacts:
President: Marco Lendi, E-mail: marco.lendi@swan.ch
Secretary: Tapio Werder, E-mail: tapio.werder@waesseri.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. Michael Hiegemann, General Electric (Switzerland) GmbH, Baden, Switzerland, E-Mail: michael.hiegemann@ge.com
Dr. Robert Svoboda, Svoboda Consulting, Wettingen, E-Mail: r.l.svoboda@swissonline.ch

Marco Lendi, Swan Analytical Instruments, Hinwil, E-Mail: marco.lendi@swan.ch
Tapio Werder, PowerPlant Chemistry Journal, Hinwil, E-Mail: tapio.werder@waesseri.com

Research activities in the reporting period:
No new projects were reported

Contributions to current IAPWS activities:
Vice-chairman of Subcommittee on Sea-Water: M. Hiegemann
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 2019 to find new participating institutions in Switzerland.
- It is therefore requested to extend the Associate Membership for another term.

M. Lendi, September 2018

U.S. National Committee to IAPWS
2018 Report on Activities of Potential Interest to IAPWS

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

- In collaboration with the Ruhr University of Bochum (Germany), we completed a new reference equation of state for the thermodynamic properties of heavy water. A paper describing the EOS has been submitted to the *Journal of Physical and Chemical Reference Data*. Work is beginning on a related IAPWS project, in collaboration with Marc Assael (Aristotle University, Greece) and Jan Sengers (University of Maryland), to develop new transport property correlations for heavy water.

- In collaboration with K. Yoshida of the University of Tokushima, work has begun on developing an IAPWS formulation for the self-diffusion coefficient of water. So far, the low-density limit has been developed, meeting correct boundary conditions and extrapolating reasonably to high and low temperatures. Dr. Yoshida has prepared a comprehensive collection of experimental data, and a preliminary classification into primary and secondary sources has been made.

- In collaboration with researchers at Fondazione Bruno Kessler (Italy), Nicolaus Copernicus University (Poland), and the University of Delaware (USA), two state-of-the-art flexible models for the water pair potential have been used to calculate second virial coefficients $B(T)$ for both H_2O and D_2O. The calculations use the path-integral Monte Carlo method, which fully accounts for both intermolecular and intramolecular quantum effects. The results agree with experimental data, but cover a wider range of temperatures; the best quantitative accuracy is achieved with the CCpol-8sf flexible model. The effect of molecular flexibility is small, but it is still significant in comparison to the uncertainty of the calculations and of the experimental data, implying that the rigid models often used for water are insufficient if the best quantitative accuracy is desired. The results for D_2O served as input for the new IAPWS EOS for heavy water.

  Path-integral calculations were also performed for the third virial coefficient $C(T)$ for both H_2O and D_2O, which requires state-of-the-art 3-body potentials (calculations with only the pair potential are qualitatively incorrect for water). Both flexible and rigid 3-body potentials were employed. While qualitative agreement with experiment was obtained, it was concluded that existing 3-body potentials are not adequate to enable quantitative prediction of $C(T)$.

  A paper describing these quantum virial calculations has been accepted in *Faraday Discussions*, DOI: 10.1039/C8FD00092A.

- Members of the Division were organizers and played major roles in the 20th Symposium on Thermophysical Properties held in Boulder in June of 2018. The conference included a number of sessions on *Properties of Aqueous Systems* organized by IAPWS Working Group members, and technical reports of potential interest to IAPWS in other sessions. The full technical program is at www.thermosymposium.nist.gov/program.html.

Communicated from the University of Maryland, College Park

- Prof. Jan Sengers continues work on the viscosity of heavy water as leader of the IAPWS task group and in conjunction with International Association for Transport Properties. A progress report will be presented at the 2018 IAPWS meeting.

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

Work has continued on an update to the document: *Consensus on Operating Practices for the Control of Feedwater and Boiler Water Chemistry in Modern Industrial Boilers.* We have also continued working on the steam/water cycle equipment inspection guidelines series. The project will consist of a series of guideline pamphlets each focused on a specific piece of equipment in the steam/water cycle and will provide the user with information on how to plan for, conduct, and interpret the results of inspections. The guidelines are 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 2018 the conference is in Scottsdale Arizona and the session titles are 1. *Water Treatment for Combined Cycle Plants* and 2. *Controlling Corrosion and Impurities in Steam and Process Condensate for Industrial Cogeneration Plants.*

Communicated from OLI Systems

- **Aqueous solution chemistry of rare-earth elements**

OLI Systems continued its participation in the Department of Energy's Critical Materials Institute (CMI). OLI's work is focused on modeling the properties of aqueous systems containing rare earth elements and providing simulation support to other members of CMI in the research on diversifying the supply, recycling, and developing substitutes for critical materials. Recent work focused on the properties of aqueous systems and solid phases containing sulfates, phosphates, chlorides, carbonates and organic complexes of rare earth elements. The recent work has been published in the following papers:

> G. Das, M.M. Lencka, A. Eslamimanesh, A. Anderko, and R.E. Riman, "Rare-Earth Elements in Aqueous Chloride Systems: Thermodynamic Modeling of Binary and Multicomponent Systems in Wide Concentration Ranges," Fluid Phase Equilibria, 452 (2017) 16-57
>
> P. Kim, A. Anderko, A. Navrotsky, R. Riman, "Trends in Structure and Thermodynamic Properties of Normal Rare Earth Carbonates and Rare Earth Hydroxycarbonates," Minerals, 8(3) (2018) 106

- **Aqueous chemistry for carbon capture technologies**

In collaboration with SRI International, OLI worked on developing simulation technology for CO_2 capture using mixed-salt (i.e., $NH_3 + K_2CO_3 + H_2O$) working fluids. A thermodynamic model has been constructed and, subsequently, process simulation studies have revealed the advantages of this technology with respect to energy requirements. This work has been summarized in the following paper:

> I. Jayaweera, P. Jayaweera, P. Kundu, A. Anderko, K. Thomsen, G. Valenti, D. Bonalumi, and S. Lilla, "Results from Process Modeling of the Mixed-Salt Technology for CO_2 Capture from Post-Combustion Related Applications," Energy Procedia, 114 (2017) 771-780.