AUSTRALIAN ASSOCIATION FOR THE PROPERTIES OF WATER & STEAM

AUSAPWS Report to IAPWS Executive Committee 2023

AUSAPWS held a three-day symposium in Melbourne from 14-16 August 2023. This was the first in-person event since 2019 and attracted more than 70 delegates from power stations, major industry, sponsors and vendors. Of particular interest to attendees was the IAPWS workshop on film-forming substances presented by David Addison.

Membership of AUSAPWS has grown to almost 100 active members (centered on power generation) and we expect to reach 150 members during 2024. Involvement with AUSAPWS is gaining recognition amongst managers and employers as an effective source of practical training and professional development for technical staff.

Alongside this increase in activity AUSAPWS has restarted its sponsorship and fundraising activities (paused in 2020) which will allow support for more frequent events for members.

Strategies goals for AUSAPWS in 2024 are:

1. To attract new members from academic and research sectors and explore ways to support basic research of interest to our members

2. To build an Australian presence in IAPWS Working Groups beyond the PCC

3. To support the hosting of satellite meetings of AUSAPWS members and build toward the next multi-day symposium in 2025

4. To maintain a healthy financial position that supports innovation in the services provided to members

Czech Society for the Properties of Water and Steam
Annual Report 2023

Submitted to IAPWS Executive Committee, November 2023

Steering board of CZPWS
Chair: Jan Hrubý (Institute of Thermomechanics of the Czech Academy of Sciences - IT CAS, hruby@it.cas.cz), Vice-Chair: Milan Sedlář (SIGMA Research and Development Institute), Secretary: Ondřej Bartoš (Czech Technical University in Prague), Member: Adam Nový (Doosan Škoda Power, s. r. o.), Member: Vladimír Majer (Technical University of Liberec).
CZPWS Meetings
Annual meeting of the CZPWS was held on June 16, 2023. The form of the meeting was hybrid. CZPWS members were informed about the activities of CZPWS Chair and approved CZPWS Financial Statements. CZPWS is a member of the Council of Scientific Societies of the Czech Republic (CSSCR). Member fee for 2023 and future CZPWS Member Dues to IAPWS will be paid based on the CZPWS membership in CSSCR. The meeting was followed by a symposium with scientific presentations by Prof. Jiří Kolafa, Prof. Josef Šedlbauer, Dr. Ondřej Bartoš, and Dr. Jan Hrubý. Ad-hoc lecture on nucleation of gas hydrates were organized at IT CAS in connection with a visit of Dr. Bernd Rathke (Univ. Bremen). A one-day symposium on thermophysical properties was organized at IT CAS with guests from TU Dresden, TU Chemnitz and Univ. Bochum).
Research
Recent data on surface tension of aqueous mixtures including the temperature range under the metastable supercooled state were presented on two international events [1,2]. The Prague team collected new data on systems with ethylene glycol and is currently performing measurements of low-concentration mixtures with methanol exhibiting a rapid drop in surface tension with increasing methanol concentration. The results of joined collaboration with the Ruhr University Bochum and the Technical University Dresden on the modeling of gas hydrates were introduced at the Prague conference held under the Czech Presidency of the Council of the European Union [3]. Research of nucleation of droplets in gaseous mixtures of water with various gases continued by a study with a sequence of gases with increasing number of atoms in the molecule: argon, nitrogen, and nitrous oxide[4] Jan Hrubý collaborated with Allan Harvey and Karsten Meier on the review paper of IAPWS activities concerning thermophysical properties of water [5].
References
1. Vinš, Václav - Součková, Monika - Čenský, Miroslav - Prokopová, Olga - Aminian, Ali - Blahut, Aleš - Hrubý, Jan: Surface tension of binary aqueous mixtures with ethylene glycol and sodium chloride including metastable supercooled state. 13th Asian Thermophysical Properties Conference (ATPC2022), pp. 202. September 26. to 30. 2022, Sendai (Japan).

2. Vinš, Václav - Součková, Monika - Blahut, Aleš - Čenský, Miroslav - Prokopová, Olga - Aminian, Ali - Hrubý, Jan: Surface tension and density of aqueous systems under the

supercooled metastable state. WORKSHOP - RESEARCH TRAINING GROUP 2430 – Interactive Fiber Rubber Composite, November 8. and 9. 2022, Lingnerschloss, Dresden (Germany).

3. Vinš, Václav - Jäger, A. - Fiedler, F. - Hrubý, Jan - Čenský, Miroslav - Span, R.: Phase Behavior of CO2-Rich Mixtures Involving Gas Hydrates and Ices as a Challenge for the Design of CCS/U Technologies. DECARB 2022 – Decarbonisation of Energy Intensive Industries – Conference under the Czech Presidency of the Council of the European Union. 10. & 11.11.2022, Prague (Czechia).

4. Lukianov, Mykola – Lukianova, Tetiana – Hrubý, Jan: Homogeneous water nucleation in argon, nitrogen, and nitrous oxide as carrier gases
   J. Chem. Phys. 158, 124301 (2023) https://doi.org/10.1063/5.0138794
5. Harvey, Allan - Hrubý, Jan - Meier, Karsten: Improved and Always Improving: Reference Formulations for Thermophysical Properties of Water.
   Journal of Physical and Chemical Reference Data 5 (2023) 011501
   https://doi.org/10.1063/5.0125524

GSAPWS to IAPWS Executive Committee

Research Activities on the Properties of Water and Steam of the German-Swiss Association for the Properties of Water and Steam (GSAPWS) e.V. in the Period 2021/2023

https://gsapws.org

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

Second Chair: Michael Rziha
PPCHEM AG, Hinwil, Switzerland

Deputy Chair: Prof. Dr. Karsten Meier
Helmut Schmidt University, Hamburg, Germany

Deputy Chair: Tapio Werder
PPCHEM AG, Hinwil, Switzerland

The Founding Assembly of the German-Swiss Association for the Properties of Water and Steam (GSAPWS) took place at the German Research Centre for Geosciences (GFZ) in Potsdam, Germany on 1 April 2022.

The second general meeting and the annual meeting of the association and took place at SWAN Analytical Instruments AG and PPCHEM AG in Hinwil, Switzerland on 20 and 21 April, 2023.

In the following, activities of certain members of the German-Swiss Association for the Properties of Water and Steam in the years 2021 to 2023 are summarized.

Baltic Sea Research Institute, Warnemuende Dr. Rainer Feistel

Recent Publications

- Hellmuth, O.; Feistel, R.; Foken, Th.:
Intercomparison of different state-of-the-art formulations of the mass density of humid air.
Bulletin of Atmospheric Science and Technology 2, 13 (2021),
https://doi.org/10.1007/s42865-021-00036-7.

- Feistel, R.; Hellmuth, O.:
Relative Humidity: A control valve of the steam engine climate.
Journal of Human, Earth, and Future 2, 139-182 (2021),
http://dx.doi.org/10.28991/HEF-2021-02-02-06.

- Feistel, R.; Hellmuth, O.; Lovell-Smith, J.:
Defining relative humidity in terms of water activity: III. Relations to dew-point and frost-point temperatures.
Metrologia 59 (2022) 045013 (27pp),
https://doi.org/10.1088/1681-7575/ac7185.

- Feistel, R.; Hellmuth, O.:

Thermodynamics of evaporation from the ocean surface. Atmosphere 14 (2023), 560 (32pp), https://www.mdpi.com/journal/atmosphere.

- Feistel, R.; Hellmuth, O.:

Non-equilibrium entropy and enthalpy of seawater evaporation. Short Note. ResearchGate Preprint, dated 11 April 2023

- Hellmuth, O.; Spänkuch, D.; Feistel, R.; Görsdorf, U.; Schwartz, S. E.:

Microphysical, optical, and thermodynamic constraints defining a warm cloud. A contribution to the discussion "What is a cloud?".
In preparation.

- Feistel, R.; Hellmuth, O.:
  Irreversible Thermodynamics of Seawater Evaporation.
  To be submitted to the Journal of Marine Science and Engineering
- Ebeling, W.; Feistel, R.; Krienke, H.:
  Statistical theory of individual ionic activity coefficients of electrolytes with multiple – charged ions including seawater.
  Journal of Molecular Liquids 346 (2022) 117814,
  https://doi.org/10.1016/j.molliq.2021.117814.
- Ebeling, W.; Feistel, R.; Grigo, M.:
  Onsager - Fuoss' matrix theory of conductivity of electrolytic mixtures applied to seawater.
  (*Dedicated to the 120th anniversary of Lars Onsager*).

In preparation.

- Ebeling, W.; Feistel, R.; Haß, E.-C.; Plath, P.:
  Zu Problemen der mechanisch – chemisch – elektrischen Energiewandlung und des Transports hochwertiger Energie im Kontext des Klimawandels.
  (*Zum Leibniztag 2023 dem Andenken an Lutz-Günther Fleischer (1938 – 2023) gewidmet, der einer der ersten Dozenten für irreversible Prozesse in Deutschland und langjähriger Vizepräsident der Leibniz – Sozietät war*).
  Submitted to Leibniz Online, August 2023.
- Hagen, E.; Feistel, R.:

Sub-surface current meanders along the Namibian shelf. Deep–Sea Research I, 167, (2021), 103432,
https://doi.org/10.1016/j.dsr.2020.103432.

- Feistel, R.:
  On the Evolution of Symbols and Prediction Models. Biosemiotics April 2023,
  https://doi.org/10.1007/s12304-023-09528-9.

GFZ German Research Centre for Geosciences
Section 4.8 – Geoenergy, Potsdam
Dr. Harald Milsch, Ulrike Hoffert

Projects

In the framework of the EU-H2020 Project "REFLECT" thermophysical investigations are performed on highly saline geothermal fluids:

1. In the past, aqueous solutions of NaCl, $CaCl_2$ and defined mixtures thereof were parameterized for density up to saturation, at temperatures between 293 K and 353 K, and ambient pressure. In cooperation with BRGM, France, the resulting original (ca. 550) new data points were compared with density predictions from numerical modelling using the

PHREESCALE geochemical code (Lach et al., 2016; 2017) yielding a satisfying match for geothermal applications within an error band of approximately 1%. A publication of these findings is in preparation for publication in *Geothermal Energy* (see below).

2. Geothermal fluids display a huge variability in chemical composition and salinity. The approach that is pursued at GFZ is to fill the existing data gaps systematically by determining the properties of synthetic fluids containing the main salts only, i.e. typically NaCl, $CaCl_2$, and KCl. To evaluate the error in density and viscosity that comes with neglecting the minor constituents of natural fluids, three European geothermal sites are selected that span a huge variability in salt concentration and composition. For each site, four synthetic samples are prepared and parameterized, one containing the main salts only and three others containing two dominant minor salts as pure and mixed additions to the base solution. This study is ongoing and the results will be published after completion.

Recent Publications

- Hoffert, U., Milsch, H., Lassin, A., Guignot, S., André, L., Sass, I.:

Density of pure and mixed NaCl and CaCl2 aqueous solutions at 20-80°C and 0.1 MPa. (2023) in preparation.

- Milsch, H., Hoffert, U., Kummerow, J., Lassin, A., André, L.:
  The H2020 REFLECT project: Deliverable D2.4 - Thermophysical properties of highly saline geothermal fluids.
  Potsdam: GFZ German Research Centre for Geosciences, p. 47 (2022)
  https://doi.org/10.48440/gfz.4.8.2022.008

Helmholtz Centre for Environmental Research, Magdeburg Dr. Bertram Boehrer

Project

Extending the solubility of noble gases for tracing natural waters and applying noble gas thermometry. (In collaboration with the Ruprecht-Karls University Heidelberg)
We measured solubility of noble gases from the atmosphere against temperature over the range from 25°C to 80°C and combined these measurements with previously available solubilities (0°C to 35°C). This we can provide a consistent curve for helium, neon, argon, krypton and xenon over the entire range from 0°C to 80°C at an accuracy of 2% to 3% depending on the separate noble gases.
This facilitates tracing of natural waters and noble gas thermometry in natural waters. We applied these new functions to the deep waters of Lake Kivu.

Recent Publications

- Schwenk, C.; Freundt, F.; Aeschbach, W.; Boehrer, B.:
  Extending Noble Gas Solubilities in Water to Higher Temperatures for Environmental Application.
  J. Chem. Eng. Data 2022, 67, 5, 1164–1173,
  https://doi.org/10.1021/acs.jced.2c00009.
- Schwenk, C.; Negele, S.; Balagizi, C. M.; Aeschbach, W.; Boehrer, B.:
  High temperature noble gas thermometry in Lake Kivu, East Africa.
  Science of The Total Environment, 837, 155859.

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

Project

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

Recent Publications

- Hellmann, R.; Harvey, A. H.:
  First-Principles Diffusivity Ratios for Atmospheric Isotope Fractionation on Mars and Titan.
  J. Geophys. Res. Planets 126, e2021JE006857 (2021).
- El Hawary, A.; Meier, K.:
  Highly Accurate Densities and Isobaric and Isochoric Heat Capacities of Compressed Liquid Water Derived from New Speed-of-Sound Measurements.
  Int. J. Thermophys., to be submitted (2023).
- Hellmann, R.:
  Cross Second Virial Coefficient of the H_2O–CO System from a New *Ab Initio* Pair Potential. Int. J. Thermophys. 43, 25 (2022).
- Huber, M. L.; Perkins, R. A.; Assael, M. J.; Monogenidou, S. A.; Hellmann, R.; Sengers, J. V.:
  New International Formulation for the Thermal Conductivity of Heavy Water.
  J. Phys Chem. Ref. Data 51, 013102 (2022).
- Harvey, A. H.; Hrubý, J.; Meier, K.:
  Improved and Always Improving: Reference Formulations for Thermophysical Properties of Water.
  J. Phys Chem. Ref. Data 52, 011501 (2023).
- Hellmann, R.:
  Cross Second Virial Coefficients of the H_2O–H_2S and H_2O–SO_2 Systems from First Principles.
  J. Chem. Eng. Data 68, 108–117 (2023).
- Hellmann, R.:
  Cross Second Virial Coefficients of the H_2O–H_2 and H_2S–H_2 Systems from First Principles.
  J. Chem. Eng. Data, in press (2023).

Dr. Olaf Hellmuth

Recent Publications

- Hellmuth, O.; Feistel, R.; Foken, Th.:
Intercomparison of different state-of-the-art formulations of the mass density of humid air.
Bulletin of Atmospheric Science and Technology 2, 13 (2021),
https://doi.org/10.1007/s42865-021-00036-7.

- Feistel, R.; Hellmuth, O.:
Relative Humidity: A control valve of the steam engine climate.
Journal of Human, Earth, and Future 2, 139-182 (2021),
http://dx.doi.org/10.28991/HEF-2021-02-02-06.

- Foken, T.; Hellmuth, O.; Huwe, B.; Sonntag, D.:
Chapter 5: Physical Quantities. In: Foken, T. (Ed.): Springer Handbook of Atmospheric Measurements.
Springer International Publishing. Hardcover, ISBN 978-3-030-52170-7, DOI 10.1007/978-3-030-52171-4 (2021).

- Sonntag, D.; Foken, T.; Vömel, H.; Hellmuth, O.:
Chapter 8: Humidity Sensors. In: Foken, T. (Ed.): Springer Handbook of Atmospheric Measurements. Springer International Publishing. Hardcover ISBN 978-3-030-52170-7, DOI 10.1007/978-3-030-52171-4 (2021).

- Spänkuch, D., O. Hellmuth, U. Görsdorf:
What is a cloud? Toward a more precise definition. Bull.
Am. Met. Soc., E1894-E1929 (2021),
https://doi.org/10.1175/BAMS-D-21-0032.1.

- Feistel, R.; Hellmuth, O.; Lovell-Smith, J.:

Defining relative humidity in terms of water activity: III. Relations to dew-point and frost-point temperatures.
Metrologia 59 (2022) 045013 (27pp),
https://doi.org/10.1088/1681-7575/ac7185.

- Feistel, R.; Hellmuth, O.:

Thermodynamics of evaporation from the ocean surface. Atmosphere
14 (2023), 560 (32pp), https://www.mdpi.com/journal/atmosphere.

- Feistel, R.; Hellmuth, O.:

Non-equilibrium entropy and enthalpy of seawater evaporation. Short Note. ResearchGate Preprint, dated 11 April 2023.

- Hellmuth, O.; Egerer, U.; Siebert, H.; Hellmuth, O.; Sorensen, L.:

PAMARCMiP Contribution: An analytical model companion based on observations: The role of low-level jets in the advection of passive tracers in the high Arctic.
Zenodo, March 1, 2023,
https://doi.org/10.5281/zenodo.7689308.

- Egerer, U.; Siebert, H.; Hellmuth, O.; Sorensen, L. L.:

The role of a low-level jet for stirring the stable atmospheric surface layer in the Arctic. Submitted to Atmos. Chem. Phys.

- Hellmuth, O.; Spänkuch, D.; Feistel, R.; Görsdorf, U.; Schwartz, S. E.:

Microphysical, optical, and thermodynamic constraints defining a warm cloud. A contribution to the discussion "What is a cloud?".
In preparation.

PPCHEM AG, Hinwil

Tapio Werder, Michael Rziha

Following Technical Guidance Documents (TGDs) are presently in development:

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

In 2023, all current TGDs will be reviewed. Based on this, the documents are updates/revised.

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

Projects:

1. The working group 3.13 'Electrochemistry' (WG 3.13) of PTB is led by Dr. Seitz. It is part of the European metrology research project "SApHTIES". The project aims to improve the traceability of pHT measurements of seawater, a quantity needed to monitor ocean acidification due to anthropogenic CO2 emissions. Empirical equations with associated uncertainties will be developed describing pHT in dependence of salinity and temperature over ranges relevant in oceanography.
2. Furthermore, WG 3.13 is associated with SCOR Working Group 145. The aim of WG 145 is to develop a user-friendly comprehensive chemical speciation model of seawater and related natural waters. WG 3.13 has, together with the metrology institutes of the US, France and Japan, carried out new potentiometric measurements, that will be used by WG145 to characterize the thermodynamic properties and speciation in the major and minor components of seawater, and in

the aqueous buffers used to calibrate instruments for measuring pH, which includes working on an uncertainty analysis of currently available data and "Pitzer" speciation models.

3. WG 3.13 is part of the European Horizon 2020 Project MINKE. MINKE (Metrology for Integrated Marine Management and Knowledge-Transfer Network) is an Horizon 2020/INFRAIA project that brings together 16 key European marine metrology research infrastructures to coordinate their use and development and propose an innovative framework of 'quality of oceanographic data' for the different European actors in charge of monitoring and managing the EOVs (Essential Ocean Variables) and marine ecosystems. MINKE includes also research activities to some extent. In this regard, WG 31.3 establishes a measurement and calibration set-up for high pressure salinity measurements.

Publication:

- Waldmann, C.; Fischer, P. F.; Seitz, S.; Köllner, M.; Fischer, J.-G.; Bergenthal, M.; Brix, H.; Weinreben, S.; Huber, R.:
  A Methodology to Uncertainty Quantification of Essential Ocean Variables. Frontiers in Marine Science 15 (2022), Sec Ocean Observation, 9 (2022), https://doi.org/10.3389/fmars.2022.1002153.

Ruhr University Bochum

Faculty of Mechanical Engineering, Chair of Thermal Turbomachines and Aeroengines

Prof. Dr. Francesca di Mare

Projects:

1. Implementation of the Spline Based Table Lookup Method (SBTL) into the in-house code SharC for high-fidelity, scale-resolving calculations of unsteady, turbulent, condensing wet steam flows at arbitrary Wilson point pressures.
   The in-house, density-based CFD solver SharC is specifically optimized for the computation of thermodynamically complex flows as, e.g., non-equilibrium condensing wet steam (SBTL based), real gas and real gas mixtures (SBTL and Peng-Robinson based) in turbomachines and, generally, complex technologically relevant devices.
   - Extension of the non-equilibrium condensation model in terms of nucleation, droplet growth and constitutive surface tension model to predict spontaneous condensation at arbitrary Wilson point pressures.
   - Generalization of the multiphase treatment in terms of arbitrarily condensable single species gas flows to investigate potential non-equilibrium condensation in the inducer region of radial compressors for closed loop supercritical CO_2-Brayton cycles.
2. Implementation of the IAPWS-IF97 for the usage in in-house codes to calculate the thermos-physical properties of water and steam on CPU's as well as highly parallel GPU's.

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

Previous research with the flow solver SharC has focused on two-phase flow in combination with non- equilibrium condensation in wet steam at low Wilson point pressures. Preliminary results demonstrate that the monodispersed source term model is now able to calculate two-phase flow and condensation at high Wilson point pressures for wet steam and sCO2. A journal publication is currently under preparation.

Ruhr University Bochum

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

Projects:

1. Our project on hydrate formation of hydrogen and its mixtures, which is carried out in cooperation with colleagues from the Institute of Thermomechanics of the Czech Academy of Sciences in Prague and from TU Dresden, has produced some first results. The consideration of hydrogen requires an extension of the hydrate model to account for multiple occupation of cavities with up to five hydrogen molecules in large SII cavities. Preliminary results were presented at the annual GSAPWS meeting; a journal publication is under preparation. However, the performance of the hydrate model greatly benefits from accurate models of the fluid phases.
   Thus, the current water-hydrogen mixture model of the GERG-2008 is being revised with colleagues of the National Institute of Standards and Technology. A multiparameter equation of state in terms of the Helmholtz energy for tetrahydrofuran, one of the most popular promoters of hydrogen hydrates, has been developed and is submitted to an international journal [1].
2. Our work in the area of property models for CCS technologies and in particular for transport of CO_2-rich mixtures resulted in a broad involvement in processes attempting to specify characteristics of CO_2-rich mixtures for multimodal CO_2-transport. The aim is to develop a European CO_2-backbone with discrimination free access for all emitters (for which emissions can hardly be avoided in different ways). The work includes memberships in the corresponding committees of ISO, DIN and DVGW and a chair position in the expert group on CO_2 characteristics implemented by the European Commission. The results of this expert group will soon be published as Annex to the upcoming Vision Paper on CO_2 infrastructure.

Recent Publication:

[1] Fiedler, F.; Karog, J.; Lemmon, E.W.; Thol, M.:
A fundamental equation of state for fluid tetrahydrofuran.
Submitted to Int. J. Thermophysics (2023).

Technical University of Dresden

Institute of Power Engineering, Thermal Power Machinery and Plants Dr. Andreas Jäger

Projects:

1. The cooperation regarding the establishment of gas hydrate models, in particular hydrogen hydrates, with colleagues from the Institute of Thermomechanics of the Czech Academy of Sciences in Prague and from Ruhr-University Bochum is continued. TU Dresden is supporting the work, which is mainly carried out within a DFG-project by Ruhr-University Bochum with Dr. Václav Vinš from the Czech Academy of Sciences being a “Mercator Fellow” of the project.
2. Within the project “Optisyskom”, heat transfer coefficients in annular cavities in the casing of steam turbines are investigated experimentally and theoretically. A test rig is being set up for this purpose and in a first step, experiments will be performed with air and transferred to steam by using the concept of similitude. In a second step, the results will be validated by directly using steam.

Recent Publications:

Paulick, O.; Eschmann, G.; Jäger, A.; Gampe, U. (2022): Test Rig Setup for the Experimental Investigation of Heat Transfer Coefficients in Annular T-shaped Cavities in Industrial Steam Turbines.
34th Workshop Turbomachinery, September 2022, Gdansk, Poland.

Zittau/Goerlitz University of Applied Sciences Faculty of Mechanical Engineering / KCE-ThermoFluidProperties, Dresden

Prof. Dr. Matthias Kunick, Prof. Dr. Hans-Joachim Kretzschmar, Dr. Sebastian Herrmann

Projects

1. Development of fast property-calculation algorithms for water and steam in thermo-hydraulic process simulations
   - Development of the property library LibSBTL95 for water and steam considering special requirements of the thermo-hydraulic code ATHLET, developed by the German Society of Global Research for Safety (GRS), Garching. Fluid properties are extrapolable beyond physical boundaries in order to satisfy the demands of the solver algorithm in ATHLET. The library is based on IAPWS-95 and the Spline- Based Table Look-Up Method (SBTL) in order to provide high accuracy and computational efficiency.
   - Implementation and verification of the property library LibSBTL95 in ATHLET.
2. Development of fast property-calculation algorithms for gaseous mixtures of water with non-condensable gases in thermo-hydraulic process simulations:
   - Development of computationally efficient algorithms for the properties of gaseous mixtures of water vapor with Ar, CO, CO2, He, H2, N2, and O2. The mixture model combines the ideal mixing of real fluids with a residual part obtained from a virial-mixing approach or a one-fluid model.
   - Implementation and verification of the property library LibSBTL95 in ATHLET.
3. Application of the Spline-Based Table Look-Up Method (SBTL) to humid air
   - SBTL functions have been developed for water and steam as well as for dry air and the enhancement factor. These SBTL functions have been implemented into a new property library for humid air which is successfully applied at the Fraunhofer UMSICHT, Oberhausen, for the simulation of Advanced Adiabatic Compressed Air Energy Storages (AA-CAES).
4. Development of a new ASHRAE standard for calculating thermodynamic properties of moist air, ASHRAE Project SPC-213P: Method for Calculating Moist Air Thermodynamic Properties.
   - The vapor pressure and saturation temperature equations of the IAPWS-IF97 Industrial Formulation and the melting pressure equation of the IAPWS Formulation 2011 are being incorporated into the new ASHRAE Standard, Method for Calculating Moist Air Thermodynamic Properties.
5. Preparation of Chapter 1 Psychrometrics for the 2025 ASHRAE Handbook of Fundamentals.
   - Tables with values of thermodynamic properties calculated from the IAPWS-IF97 Industrial Formulation and of transport properties calculated from the IAPWS Formulation 2008 for the viscosity and the IAPWS Formulation 2011 for the thermal conductivity of water are being incorporated into the 2025 ASHRAE Handbook of Fundamentals.

Recent Publications

- Kretzschmar, H.-J.; Kraft, I.:
  Kleine Formelsammlung Technische Thermodynamik, 6. aktualisierte Auflage (Short Collection of Technical Thermodynamic Formulae, 6th Revised edition.)
  Carl Hanser Verlag München (2022).
  ISBN 978-3-446-47028-6, E-Book-ISBN 978-3-446-47321-8.
- Herrmann, S.; Kretzschmar, H.-J.; Aute, V. C.; Gatley, D. P.; Vogel, E.:
  Transport Properties of Real Moist Air, Dry Air, Steam, and Water.
  Science and Technology for the Built Environment, 27 (2021), pp. 393 - 401. DOI: 10.1080/23744731.2021.1877519.
- Herrmann, S.; Kretzschmar, H.-J.; Gatley, D.P.:
  In: 2021 ASHRAE HANDBOOK FUNDAMENTALS, SI and I-P Editions, Chapter 1 PSYCHROMETRICS,
  Table 2 Thermodynamic Properties of Moist Air at Standard Atmospheric Pressure.
  Table 3 Thermodynamic Properties of Water at Saturation.
  Table 5 Transport Properties of Moist Air at Standard Atmospheric
  Pressure. Table 6 Transport Properties of Water at Saturation.
  American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA (2021)
  I-P-Version: ISBN: 978-1-947192-89-8, ISSN: 1523-7222
  SI-Version: ISBN: 978-1-947192-90-4, ISSN: 1523-7230
- Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.;
  Friend, D. G.; Harvey, A. H.:
  Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL).
  J. Eng. Gas Turbines Power, in preparation.

Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, September, 2023

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

I. Overview:

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

II. Recent Publications:

Yasuoka, Kenji
Professor, Department of Mechanical Engineering, Keio University
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Report on IAPWS Annual Meeting 2022
K. Yoshida, K. Yasuoka
The Thermal and Nuclear Power, (in press, in Japanese)

Learned pseudo-random number generator: WGAN-GP for generating statistically robust random numbers
K. Okada, K. Endo, K. Yasuoka, S. Kurabayashi
PLOS One, 18, e0287025 (19 pages), 2023

Wetting hysteresis induces effective uni-directional water transport through a fluctuating nanochannel
N. Arai, E. Yamamoto, T. Koishi, Y. Hirano, K. Yasuoka, T. Ebisuzaki
Nanoscale Horiz., in press. (12 pages) DOI : 10.1039/D2NH00563H

Combining molecular dynamics and machine learning to analyze shear thinning for alkane and globular lubricants in the low shear regime
I. Yasuda, Y. Kobayashi, K. Endo, Y. Hayakawa, K. Fujiwara, K. Yajima, N. Arai, K. Yasuoka,
ACS Appl. Mater. Interfaces, in press. (12 pages) DOI : 10.1021/acsami.2c16366

Prediction of Water Diffusion in Wide Varieties of Polymers with All-Atom Molecular Dynamics Simulations and Deep Generative Models
R. Kawada, K. Endo, K. Yasuoka, H. Kojima, N. Matubayasi
J. Chem. Inf. Model., 63, 76-86, 2022

MD-GAN with multi-particle input: the machine learning of long-time molecular behavior from short-time MD data
R. Kawada, K. Endo, D. Yuhara, K. Yasuoka,
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Y. Kobayashi, N. Arai, K. Yasuoka
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Impact of free energy of polymers on polymorphism of polymer-grafted nanoparticles
M. Ishiyama, K. Yasuoka, M. Asai
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Optimal Replica-Exchange Molecular Simulations in Combination with Evolution Strategies
A. Kowaguchi, K. Endo, P. E. Brumby, K. Nomura, K. Yasuoka
J. Chem. Inf. Model., 62, 6544-6552, 2022

Differences in ligand-induced protein dynamics extracted from an unsupervised deep learning approach correlate with protein–ligand binding affinities
I. Yasuda, K. Endo, E. Yamamoto, Y. Hirano, K. Yasuoka
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A stochastic Hamiltonian formulation applied to dissipative particle dynamics
L. Peng, N. Arai, K. Yasuoka
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Efficient Monte Carlo Sampling for Molecular Systems Using Continuous Normalizing Flow
K. Endo, D. Yuhara, K. Yasuoka
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Natural quantum reservoir computing for temporal information processing
Y. Suzuki, Q Gao, K. C. Pradel, K. Yasuoka, N. Yamamoto
Sci. Rep., 12, 1353 (15 pages), 2022

An Efficient Random Number Generation Method for Molecular Simulation
K. Okada, P. E. Brumby, K. Yasuoka
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Chain-Increment Approach to the Mutual Miscibility of Polymers with All-Atom Molecular Simulation
K. Yamada, N. Matubayasi
Macromolecules, 56, 3857-3872, 2023

Understanding Sorption Mechanisms Directly from Isotherms
S. Shimizu, N. Matubayasi
Langmuir, 39, 6113-6125, 2023

Revealing the hidden dynamics of confined water in acrylate polymers: Insights from hydrogen-bond lifetime analysis
K. Shikata, T. Kikutsuji, N. Yasoshima, K. Kim, N. Matubayasi,
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H. S. Sarkar, T. Mashita, T. Kowada, S. Hamaguchi, T. Sato, K. Kasahara, N. Matubayasi, T. Matsui, S. Mizukami,
ACS Chem. Biol., 18, 340-346, 2023

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M. Suzuki, A. Tsuchiko, Y. Tanaka, N. Matubayasi, G. Mogami, N. Uozumi, S. Takahashi,
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Prediction of Water Diffusion in Wide Varieties of Polymers with All-Atom Molecular Dynamics Simulations and Deep Generative Models
R. Kawada, K. Endo, K. Yasuoka, H. Kojima, N. Matubayasi,
J. Chem. Inf. Model., 63, 76-86, 2023

Diffusion theory of molecular liquids in the energy representation and application to solvation dynamics
K. Okita, K. Kasahara, N. Matubayasi,
J. Chem. Phys., 157, 244505 (14 pages), 2022

Cooperative Sorption on Heterogeneous Surfaces,
O. P. L. Dalby, S. Abbott, N. Matubayasi, S. Shimizu
Langmuir, 38, 13084-13092, 2022

Molecular dynamics study of the interactions between a hydrophilic polymer brush on graphene and amino acid side chain analogues in water
T. Yagasaki, N. Matubayasi
Phys. Chem. Chem. Phys., 24, 22877-22888, 2022

Constructing a Memory Kernel of the Returning Probability to Efficiently Describe Molecular Binding Processes
K. Kasahara, R. Masayama, Y. Matsubara, N. Matubayasi

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Crystal Growth of Urea and Its Modulation by Additives as Analyzed by All-Atom MD Simulation and Solution Theory
S. Tanaka, N. Yamamoto, K. Kasahara, Y. Ishii, N. Matubayasi
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Surface Area Estimation: Replacing the Brunauer-Emmett-Teller Model with the Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
Langmuir, 38, 7989-8002, 2022

Nonpolarizable Force Fields through the Self-Consistent Modeling Scheme with MD and DFT Methods: From Ionic Liquids to Self-Assembled Ionic Liquid Crystals
Y. Ishii, N. Matubayasi, H. Washizu
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Adsorption Energetics of Amino Acid Analogs on Polymer/Water Interfaces Studied by All-Atom Molecular Dynamics Simulation and a Theory of Solutions
N. Yasoshima, T. Ishiyama, N. Matubayasi
J. Phys. Chem. B, 126, 4389-4400, 2022

All-atom molecular simulation study of cellulose acetate: amorphous structure and the dissolution of small molecule
R. Matsuba, H. Kubota, N. Matubayasi
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Explaining reaction coordinates of alanine dipeptide isomerization obtained from deep neural networks using Explainable Artificial Intelligence (XAI)
T. Kikutsuji, Y. Mori, K. Okazaki, T. Mori, K. Kim, N. Matubayasi
J. Chem. Phys., 156, 154108 (8 pages), 2022

Anion-cation contrast of small molecule solvation in salt solutions
S. Hervø-Hansen, J. Heyda, M. Lund, N. Matubayasi
Phys. Chem. Chem. Phys., 24, 3238-3249, 2022

Simulating the nematic-isotropic phase transition of liquid crystal model via generalized replica-exchange method
K. Takemoto, Y. Ishii, H. Washizu, K. Kim, N. Matubayasi
J. Chem. Phys., 156, 014901 (8 pages), 2022

Ensemble transformation in the fluctuation theory
S. Shimizu, N. Matubayasi
Physica A, 585, 126430 (14 pages), 2022; Physica A, 605, 127987 (1 pages), 2022

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Report on IAPWS Annual Meeting 2022
K. Yoshida, K. Yasuoka
The Thermal and Nuclear Power, (in press, in Japanese)

Nuclear Magnetic Resonance Analysis of Hydrothermal Reactions of Ethyl- and Octylamine in Sub- and Supercritical Water
K. Yoshida, A. Doi, H. Yoshioka, T. Hirano, M. Nakahara
J. Phys. Chem. A, 127, 3848-3861, 2023

Significant role of counterion for lead(II) ion adsorption on carbon pore surface
T. Horikawa, M. Okamoto, A. Kuroki-Matsumoto, K. Yoshida
Carbon, 196, 575-588, 2022

Structure and Formation Mechanism of Protective Coatings on Steam Piping Composed of Film-Forming Amines
K. Yoshida
The Thermal and Nuclear Power, 73, 32-39, 2022 (in Japanese)

Microscopic Structure and Binding Mechanism of the Corrosion-Protective Film of Oleylpropanediamine on Copper in Hot Water
H. Yoshioka, K. Yoshida, N. Noguchi, T. Ueki, K. Murai, K. Watanabe, M. Nakahara
J. Phys. Chem. C, 126, 6436-6447, 2022

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Nuclear Magnetic Resonance Analysis of Hydrothermal Reactions of Ethyl- and Octylamine in Sub- and Supercritical Water
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H. Yoshioka, K. Yoshida, N. Noguchi, T. Ueki, K. Murai, K. Watanabe, M. Nakahara
J. Phys. Chem. C, 126, 6436-6447, 2022

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Volume transport of the Kuroshio south of Japan estimated from repeated full-depth hydrographic surveys and current measurements
S. Imawaki, H. Uchida, H. Ichikawa, M. Fukasawa, S. Umatani, H. Yoritaka
J. Oceanogr. 79, 175-183, 2022

Source analysis of dissolved methane in Chukchi Sea and Bering Strait during summer – autumn of 2012 and 2013
K. Kudo, S. Toyoda, K. Yamada, N. Yoshida, D. Sasano, N. Kosugi, A. Murata, H. Uchida, S. Nishino
Mar. Chem., 243, 104119, 2022

Miyamoto, Hiroyuki
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Measurements and Modeling of the Vapor–Liquid Equilibrium Properties of Low-Global-Warming-Potential Refrigerant R32/R1234yf/R1123 Ternary Mixtures
H. Miyamoto, Y. Nakamura, K. Minai, T. Yamada
Fluid Phase Equilib., 558, 113440 (11 pages), 2022

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Semi-Quantitative Microfluidic Paper-Based Analytical Device for Ionic Silica Detection
M. Ogawa, A. Katoh, R. Matsubara, H. Kondo, M. Otsuka, T. Sawatsubashi, Y. Hiruta, D. Citterio
Anal. Sci., DOI: 10.1007/s44211-023-00345-1, 2023

Semi-quantitative Microfluidic Paper-based Analytical Device for Ionic Silica Detection
M. Ogawa, A. Katoh, R. Matsubara, H. Kondo, M. Otsuka, T. Sawatsubashi, Y. Hiruta, D. Citterio
Royal Society of Chemistry Tokyo International Conference 2022 (RSC-TIC2022)

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Hydrogen Damage in Power Boiler: A Study of Damage Selectivity and Conditions
T. Ichihara, Y. Amano, M. Machida
Eng. Fail. Anal., 143, 106842, 2023

Hydrogen Damage in a Power Boiler: Correlations between Damage Distribution and Thermal-Hydraulic Properties

T. Ichihara, R. Koike, Y. Watanabe, Y. Amano, M. Machida
Eng. Fail. Anal., 146, 107120, 2023

Study of Hydrogen Damage in Boiler Evaporator Tube: Damage Selectivity and Conditions
T. Ichihara
Chiba University, Ph. D. thesis, 2023 (in Japanese)

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Novel Identification Method of Seawater Contamination into Steam-Water Circuit Including Carbon Dioxide of Power Plants based on pH, Specific Conductivity, and Cation Conductivity Y. Nakatsuchi, A. Hamasaki, H. Kido, T. Iwato
J. Chem. Eng. Japan, in press

New Proposal of Water Quality Management for Gas Turbine Combined Cycle Plant
Y. Nakatsuchi, A. Hamasaki, H. Kido, T. Iwato
Therm. Nucl. Power, 73, 869-876, 2022 (in Japanese)

Novel Prediction Model Based on Two-Film Theory for Ammonia Distribution Coefficient in Heat Recovery Steam Generator of Gas Turbine Combined Cycle Power Plants
Y. Nakatsuchi, H. Kido, A. Hamasaki, S. Fujimoto
J. Chem. Eng. Japan, 55, 281-289, 2022

III. Presentations at JPAPWS General Meetings:

FY2022 1st General Meeting, May 31, 2022

Radiation chemistry in reactor water of boiling water reactors
Youichi Wada（Hitachi, Ltd.）

Status of Geothermal Power Generation in the World
Shigeto Yamada（Fuji Electric Co.,Ltd.）

FY2022 2nd General Meeting, October 21, 2022

Hydrogen Damage in Power Boiler: A Study of Damage Selectivity and Conditions
Taro Ichihara (Mitsubishi Heavy Industries Power IDS, Ltd.)

Strategies to improve criteria on steam for steam turbine
Shin-ichi Terada (Toshiba Energy Systems & Solutions Corporation)

Crystal Growth of Urea and Its Modulation by Additives as Analyzed by All-Atom MD Simulation and Free-Energy Calculation
Nobuyuki Matubayasi (Osaka University)

Research Trends and Issues Concerning Film-Forming Amines
Ken Yoshida (Tokushima University)

FY2022 3rd General Meeting, January 27, 2023

Global Trends for Film-forming Corrosion Inhibitors in Water-steam Cycle
Shuichi Tachibana (Aquas Co., Ltd.)

FY2022 4th General Meeting, March 20, 2023

Innovative Next-Generation Reactors and Hydrogen Production Technology toward Carbon Neutrality
Takeshi Matsuo（Mitsubishi Heavy Industries, Ltd.）

FY2023 1st General Meeting, May 30, 2023

Research background and the current status of the JPAPWS research grant: Thermodynamic properties evaluation on metastable state for heavy water
Yohei Kayukawa (AIST)

FY2023 2nd General Meeting, July 25, 2023

NMR analysis of hydrothermal reactions of ethylamine and octylamine
Ken Yoshida (Tokushima University)

Comparison of experimental and calculated ionization constants for subcritical/supercritical water
Masaru Nakahara (Kyoto University), Ken Yoshida (Tokushima University)

Present status of the absolute density measurements for sea-water
Yohei Kayukawa (AIST)

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

NEW ZEALAND Association for the Properties of WATER & STEAM

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

Date: 7 September 2023, Rev 1.1

Key Achievements:

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

2. Successfully arranged and hosted the 2022 IAPWS in person meeting in Rotorua, New Zealand from 27th to 2nd December 2022. The Symposium attracted over 60 attendees and the Workshop over 113 with full week attendees numbering 33. The meeting was financially successful covering all NZAPWS expenses.

INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER & STEAM IAPWS ANNUAL MEETING 2022 ROTORUA, NEW ZEALAND 27TH NOVEMBER – 2ND DECEMBER

3. NZAPWS has robust funding in place and has gained additional sponsors for the 2022/2023 year as part of the IAPWS2022 and is in a good financial position

4. NZAPWS has an active membership covering the following areas:
    a. Fossil power generation
    b. Industrial steam production and use for dairy product production
    c. Geothermal power generation (subsurface and surface operations)
    d. Humidity research and services
    e. Water/steam analytical services
    f. Water/steam chemical treatment and services
    g. Electrode/electrical resistance boilers (**Note**: new area of interest for NZ and IAPWS as these plants have started to be installed in NZ to replace existing industrial coal boilers and have presented significant water/steam issues)

5. NZAPWS have a dedicated website – www.nzapws.org.nz to provide relevant information and to manage meetings for NZAPWS

Key Activities:

1. IAPWS 2022 NZ meeting very successful

2. NZAPWS have been supporting the AUSAPWS 2023 meeting

3. Next NZAPWS meeting to be in 2024 (skipped 2023)

4. David Addison has had ongoing involvement in a PCC IAPWS International Collaboration project with the University of New Brunswick (DR Willy Cook) working on high temperature electrochemical corrosion monitoring – Covid has prevented any follow up visits to UnB

5. David Addison and Ian Richardson have continued working on geothermal related aspects for a IAPWS white paper along with Nobuo Okita (Toshiba) of Japan. Work is ongoing

6. David Addison has worked on electrode boiler water/steam chemistry issued in conjunction with SIAPWS members (Karsten Thompson and Monica Nielsen) sharing experiences and learnings with various different electrode boiler makes and models

7. Jeremy Lovell-Smith has had ongoing involvement in TPWS and SCW and intends to continue to be actively involved (but unable to attend IAPWS 2023)

Publications:

None for 2023 at this stage

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SIAPWS
ALL ABOUT WATER

Scandinavian International Association on the Properties of Water and Steam

SIAPWS Report to IAPWS Executive Committee 2023

SIAPWS consists of one Nordic Executive Committee bringing the Nordic countries together around the topic of water and steam and in each country Denmark, Sweden and Finland national groups are formed. In both Denmark and Finland, we have around 40 company members and in Sweden around 120 company members, so in total around 200 members.

Our members are among others from the following industries:

a. Fossil / biomass power generation
b. Boiler manufactures.
c. Waste incineration
d. Industrial steam production (pulp and paper)
e. Water treatment suppliers
f. Suppliers of analytical instruments
g. Consulting companies
h. Electrode/electrical resistance boiler manufactures.
i. Laboratories
j. Universities and Institutes

In March 2022 we held the annual general meeting and workshop in Uppsala, Sweden attracting around 30 people for a 1½ day workshop and plant visit.
Each National group have their own annual meetings and workshops during the year.

Next year the SIAPWS Nordic annual meeting and workshop will be held in Oslo, Norway on the 14.-15. March 2024. SIAWS only have very few members from Norway, and the aim of the event is to attract more members from Norway and in the end to create a national group in Norway. The topics for this meeting will be general around IAPWS and introducing the working groups of IAPWS and the Releases, Guidelines and ICRNs and some technical presentations.

In 2023 up until now, SIAPWS has hosted three webinars on the topics: FAC, SWAS systems and Dosing System. In the Fall another three webinars are planned for September, October, and November on the topics: Chemical cleaning of new boilers, Experiences with the counter current flushed MBR and Industrial wastewater treatment. We typically have between 30-40 participants at these webinars.

SIAPWS EC has been in Helsinki in August 2023 where we started the planning of the IAPWS Annual Meeting in 2025.

In the Danish National Group, we are working on understanding the chemistry in electrical boilers and we have established a Danish Electrical Boiler Working Group which meet every or every second year for exchange of experience. This year we are meeting on September 12 and this time we have invited the electrical boiler manufactures in Denmark.

Monika Nielsen, SIAPWS Chair

U.S. National Committee to IAPWS
2023 Report on Activities of Potential Interest to IAPWS

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

A collaboration between NIST and the group of Prof. Tremaine at the University of Guelph has the objective of developing a standard formulation for the static dielectric constant of heavy water. Thus far, we have gathered the available data and made preliminary comparisons based on the existing H_2O correlation in order to see where there are gaps in the data that might need to be filled in based on H_2O behavior. It is hoped that a new formulation will be ready before the 2024 IAPWS meeting.

In collaboration with G. Garberoglio (Italy), calculations have been performed with state-of the-art surfaces from the literature to characterize the different contributions to the first dielectric virial coefficient of water. This includes the electronic and vibrational polarizabilities, the dipole moment, and the rotational quantum effects that cause the dielectric behavior to deviate from the classical Debye expression. A paper is pending (G. Garberoglio, C. Lissoni, L. Spagnoli, and A.H. Harvey, "Comprehensive Quantum Calculation of the First Dielectric Virial Coefficient of Water," in preparation (2023)).

A review article has been published on the thermophysical properties of water, with an emphasis on IAPWS formulations: A.H. Harvey, J. Hrubý, and K. Meier, "Improved and Always Improving: Reference Formulations for Thermophysical Properties of Water," *Journal of Physical and Chemical Reference Data* **52**, 011501 (2023).

Communicated from OLI Systems Inc., Parsippany, NJ:

Aqueous chemistry of critical materials

Under the auspices of the Department of Energy's Critical Materials Institute, OLI Systems continued its work on the aqueous chemistry of critical materials including rare earth elements and lithium-ion battery cathode materials. The recent work was focused on (1) development of simulation methodology to predict the behavior of rare earths in the presence of inorganic and organic ligands and (2) modeling the thermodynamics of reactive systems used for the recovery of metals from spent lithium-ion battery cathodes using biological media. The results of the work on project (1) have been published in the following paper:

> G. Das, M.M. Lencka, J. Liu, A. Anderko, R.E. Riman, and A. Navrotsky, "Modeling phase equilibria and speciation in aqueous solutions of rare earth elements with hydroxide and organic ligands," *J. Chem. Thermodynamics* **186** (2023) 107125.

The results of project (2) have been summarized in the following paper, which has been submitted for publication in *Resources, Conservation and Recycling*:

M. Alipanah, H. Jin, Q. Zhou, C. Barboza, D. Gazzo, V. Thompson, Y. Fujita, J. Liu, A. Anderko, and D. Reed, "Sustainable Bioleaching of Lithium-ion Batteries for Critical Materials Recovery: Process Optimization through Design of Experiments and Thermodynamic Modeling."

Aqueous chemistry of boric acid and borates up to high temperatures

In collaboration with Professor Tremaine of the University of Guelph, we have completed a comprehensive study of the speciation and solubility of boric acid and various borates (i.e., lithium, sodium, potassium, calcium, magnesium and zinc borates) ranging from ambient to high temperatures. While the low- and moderate-temperature behavior of these systems is important for the supply and separation of materials in the mining industry, the high-temperature behavior is important for nuclear power generation. The work has been described in the following paper, which has been submitted for publication:

P. Wang, A. Anderko, and P.R. Tremaine, "Speciation and phase equilibria of aqueous boric acid and alkali metal borates from ambient to hydrothermal conditions: a comprehensive thermodynamic model."

Communicated from Idaho National Laboratory, Idaho Falls, ID:

Successful demonstration of a custom-built high temperature (up to 200 ^{o}C) titanium cell for cobalt-60 irradiations of aqueous solutions with *in-situ* UV-Vis spectroscopy via coupled fiber optics was achieved. This custom-made device was used for monitoring the high temperature radiation-induced behavior of key alloying metal ions (chromium and iron) in aqueous solutions in real time. To my knowledge, these are the first *in-situ* irradiation studies of this kind to be performed, and they provide important data for benchmarking multiscale models of these chemical systems.