Czech Society for the Properties of Water and Steam

Annual Report 2024

Submitted to IAPWS Executive Committee, June 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 18, 2024. 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 2024 and, expectedly, 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 Aleš Blahut, Václav Vinš, and Jan Hrubý.

Research

In collaboration with the Ruhr University Bochum and the Technical University Dresden, the van der Waals and Platteeuw model for gas hydrates combined with the multiparameter EoSs, including IAPWS-95 formulation for water, has been successfully extended to account for a multiple cage occupancy of water cavities by gas molecules [1]. This is important especially for accurate modeling of hydrogen hydrates showing up to quadruple occupancy of the large cavities in the crystal structure sII. At 22nd European Conference on Thermophysical Properties, the IT CAS team has presented new experimental data for the surface tension of aqueous mixtures with methanol including the temperature range under the metastable supercooled state [2].

At IT CAS, Jan Hrubý continued in the development of a new mixture model, applicable to contemporary Helmholtz energy models, which is consistent with the rigorous mixing rules for virial coefficients. Published results [3] include general formulation of the model, virial expansion up to 4^{th} degree, and finding that a simple variant of the model gives identical results when applied to a two-parameter cubic equation of state as the standard approach using van der Waals mixing rules. Further work (to be reported at 18^{th} ICPWS in Boulder) included predictive computations of thermodynamic properties and phase equilibria for simple fluid mixtures, which proved to be successful. It turned out, however, that modeling vapor-liquid phase equilibria (VLE) and states close VLE requires that the equations of state show single van der Waals loop between saturated vapor and saturated liquid densities. The present multiparemeter equations of state, including IAPWS-95, exhibit multiple van der Waals loops. Consequently, it appears highly desirable that the future fundamental formulation of the properties of ordinary water shows a single van der Waals loop and it is as much as possible supported by experimental data and molecular simulations in the metastable vapor and liquid regions.

The problems studied in the SIGMA Research and Development Institute and the Centre of Hydraulic Research in the period of June 2023 – June 2024 have been related mainly to the modelling of cavitation erosion during the hydrodynamic cavitation and to the thermal effects of

cavitation and the exact description of water and water vapour properties during the cavitation flows. In cooperation with the Institute of Physics/Czech Academy of Sciences, the tests of cavitation resistance of steel samples treated with Laser Shock Pealing (LSP) and 3D printed samples with different surface patterns have continued from the last two years. The cavitation erosion stand has been reconstructed for higher speeds and equipped with the transparent lid enabling continuous monitoring by cameras. These tests have been accompanied by advanced numerical simulations. Some experimental and simulation results will be presented in the 5th International Symposium on Thermal-Fluid Dynamics (ISTFD 2024), Xi'an, China, July 26 – 29, 2024 [4]. Concerning the thermal effects of cavitation, a new hot water cavitation tunnel (Venturi type) has been designed and put into the production phase. It is equipped with two sapphire windows which will enable to measure in the infra-red spectrum. Supporting simulations of cavitating flow in the temperature range of 25 – 175 °C have been performed to confirm the functionality and design parameters.

Adam Nový (Doosan-Skoda Power) continued in activities relevant to RIS WG, in particular:

- validation procedure for IF97 implementations in other programing languages than Fortran,
- discussion on future steam properties formulation,
- discussion of strategy to support proposal of Spline-Based Table Look-Up Method (SBTL) as new IAPWS release.

References

1. Fiedler, F., Vinš, V., Jäger, A., Span, R.: Modification of the van der Waals and Platteeuw model for gas hydrates considering multiple cage occupancy. Journal of Chemical Physics. Roč. 160, č. 9 (2024), č. článku 094502. ISSN 0021-9606. E-ISSN 1089-7690.

2. Vinš, V., Součková, M., Čenský, M., Prokopová, O., Hrubý, J., Blahut, A., Aminian, A.: Surface tension of low-concentration aqueous mixtures with methanol and ethylene glycol including metastable supercooled state. 22nd European Conference on Thermophysical Properties /22./. 10.09.2023-13.09.2023, Venice, s. 255-255. ISBN 9791221042207.

3. Hrubý, J: A General Model for Thermodynamic Properties of Fluid Mixtures Based on Helmholtz Energy Formulations for the Components. Virial Expansion and Reduction to van der Waals Mixing Rules. Int J Thermophys 44, 130 (2023).

4. Sedlář, M., Koutný, A., Krátký, T., Komárek, M., Fulín, M.: Prediction of Cavitation Erosion Using CFD and Bubble Dynamics Model. *Extended Abstract of 5th International Symposium on Thermal-Fluid Dynamics (ISTFD 2024)*, to be published in August 2024.

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 2023/2024

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 2024 General Meeting and the Annual Meeting of the German-Swiss Association for the Properties of Water and Steam (GSAPWS) took place at the Dresden University of Technology on 14 and 15 March, 2024.

In the following, activities of certain members of the German-Swiss Association for the Properties of Water and Steam in the years 2023 to 2024 are summarized.

Baltic Sea Research Institute, Warnemuende Dr. Rainer Feistel

Recent Publications

- McDougall, T.J., Barker, P.M., Feistel, R., Roquet, F.:
  A thermodynamic potential of seawater in terms of Absolute Salinity, Conservative Temperature, and in situ pressure.
  Ocean Sci. 19(2023), 1719–1741. https://doi.org/10.5194/os-19-1719-2023
- 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.
  Leibniz Online 50 (2023), https://doi.org/10.53201/LEIBNIZONLINE50
- Feistel, R.:
  On the Evolution of Symbols and Prediction Models.
  Biosemiotics 16 (2023), 311–371, https://doi.org/10.1007/s12304-023-09528-9
- Feistel, R. (2023):
  Self-Organisation of Prediction Models.
  Entropy 25 (2023), 1596. https://doi.org/10.3390/e25121596
- Feistel, R., Hellmuth, O.:
  Thermodynamics of Evaporation from the Ocean Surface.
  Atmosphere 14 (2023), 560. https://doi.org/10.3390/atmos14030560
- Feistel, R., Hellmuth, O.:

Irreversible Thermodynamics of Seawater Evaporation.
J. Mar. Sci. Eng. 12 (2024), 166. https://doi.org/10.3390/jmse12010166

- Feistel, R., Hellmuth, O.:
  TEOS-10 Equations for the Lifted Condensation Level (LCL) and Climatic Feedback of Marine Clouds.
  Preprints 2024031171 (2024). https://doi.org/10.20944/preprints202403.1171.v1
  submitted to "Oceans", under review
- Feistel, R.:
  TEOS-10 and the Climatic Relevance of Ocean-Atmosphere Interaction.
  EGUshere (2024), https://doi.org/10.5194/egusphere-2024-1243

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 was submitted to *Geothermal Energy* (Springer; Hoffert et al., 2024a; see below).
2. For the same set of samples at the mentioned conditions, viscosity was determined yielding a full parameterization of the extended Jones-Dole-Equation. A publication of these findings is currently in preparation and will also be submitted to *Geothermal Energy* (Springer; Hoffert et al., 2024b; see below).
3. 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, four 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

- Ulrike Hoffert, Laurent André, Guido Blöcher, Sylvain Guignot, Arnault Lassin, Harald Milsch, Ingo Sass (2024a): Density of pure and mixed NaCl and $CaCl_2$ aqueous solutions at 293 K to 353 K and 0.1 MPa: An integrated comparison of analytical and numerical data. Geothermal Energy, under review.

- Ulrike Hoffert, Guido Blöcher, Stefan Kranz, Harald Milsch, Ingo Sass (2024b): Viscosity of pure and mixed NaCl and $CaCl_2$ aqueous solutions at 293 K to 353 K and 0.1 MPa: A parameterization of the extended Jones-Dole Equation with original analytical data. Geothermal Energy, in preparation.

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

- **A. El Hawary, K. Meier:**
  Highly Accurate Densities and Isobaric and Isochoric Heat Capacities of Compressed Liquid Water Derived from New Speed of Sound Measurements
  Int. J. Thermophys. 44, 180 (2023) (Open Access).
- Hellmann, R.:
  Cross Second and Third Virial Coefficients and Dilute Gas Transport Properties of the (H_2O + Ar) System from First-Principles Calculations.
  J. Chem. Eng. Data 69, 942-957 (2024).

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

Recent Publications

- Feistel, R., Hellmuth, O.:
  Thermodynamics of Evaporation from the Ocean Surface.
  Atmosphere 14 (2023), 560. https://doi.org/10.3390/atmos14030560
- Feistel, R., Hellmuth, O.:
  Irreversible Thermodynamics of Seawater Evaporation.
  J. Mar. Sci. Eng. 12 (2024), 166. https://doi.org/10.3390/jmse12010166
- Feistel, R., Hellmuth, O.:
  TEOS-10 Equations for the Lifted Condensation Level (LCL) and Climatic Feedback of Marine Clouds.
  Preprints 2024031171 (2024). https://doi.org/10.20944/preprints202403.1171.v1
  submitted to "Oceans", under review

PPCHEM AG, Hinwil

Tapio Werder, Michael Rziha

The activities for the PCC WG were limited only to a minor contribution for the amendment / revision of the existing TGD2-09 Instrumentation for monitoring and control of cycle chemistry for the steam/water circuits of fossil-fired, combined cycle and industrial power plants.

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 has established traceability for spectrophotometric measurements of the pH_T of seawater, a quantity needed to monitor ocean acidification due to anthropogenic CO_2 emissions. WG 3.13 has developed empirical equations with associated uncertainties which can be used to assign pH_T values to primary artificial seawater standards from Harned cell measurements in dependence of salinity and temperature over ranges relevant in oceanography. A respective publication is in preparation.

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 have been used by other partners in 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. The speciation model has been published by the partners. Another publication, including the evaluation of PTB’s measurement data is in preparation.
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. Furthermore, PTB has contributed to establish links between MINKE and the European Metrology Network for Climate an Ocean Observation (see https://www.euramet.org/climate-and-ocean-observation)

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

Projects:

1. Extension of the in-house code SharC for investigations of the flow in radial turbines including its disc cavities using the Spline Based Table Lookup Method (SBTL) applied for the Span-Wagner reference equation of state.
    a. Interfaces between adjacent blade rows and between the main channel and the cavities are modeled in a highly conservative and efficient manner by using the

SBTL to compute primitive variables, such as pressure, from the enthalpy flux across cell boundaries.

b. Within the AG Turbo project DigITecT AP2.2b the extended version of the CFD solver was applied to assess the performance of a newly developed turbine stage, the role of non-ideal thermodynamic effects in the flow field and the axial thrust acting on the impeller wheel. The results will be presented on the ASME Turbo Expo 2024 in London and published in the conference preceedings[1].

Recent Publication:

[1] Lea, B.; Franz, H.; di Mare, F.:
Numerical Investigation of the axial thrust load of a prototype radial turbine for supercritical CO_2 cycles.
Proceedings of ASME Turbo Expo 2024: Turbine Technical Conference and Exposition. Paper No. GT2024-123806 (accepted).

Ruhr University Bochum
Faculty of Mechanical Engineering, Chair of Thermodynamics
Prof. Dr. Dr. h.c. 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, is approaching the end of the first project phase. The consideration of hydrogen required an extension of the hydrate model to account for multiple occupation of cavities with up to five hydrogen molecules in large SII cavities. A Journal publication explaining the way how this can be treated numerically has been published end of 2023 [1]. The performance of the hydrate model greatly benefits from accurate models of the fluid phases; a new Helmholtz mixture model for the system water / hydrogen is under development.
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, DVGW, CEN and in the expert group on CO_2 characteristics implemented by the European Commission. The results obtained by this expert group in 2023 have been published as a report by the European Commission [2]. The latest version of our mixture model for CO_2-rich mixtures, EOS-CG-2021, has been published [3].

Recent Publication:

[1] Fiedler, F.; Vinš, V.; Jäger, A.; Span, R.:
Modification of the van der Waals and Platteeuw Model for Gas Hydrates Considering Multiple Cage Occupancy.
Journal of Chemical Physics (2024), 160 (9), 094502.
https://doi.org/10.1063/5.0189555.

[2] An Interoperable CO_2 Transport Network – Towards Specifications for the Transport of Impure CO_2. Report of the CCUS Forum Expert Group on CO_2 Specifications. https://zeroemissionsplatform.eu/wp-content/uploads/An-Interoperable-CO2-Transport-Network.pdf

[3] Neumann, T.; Herrig, S.; Bell, I.; Beckmüller, R.; Lemmon, E.W.; Thol, M.; Span, R.: EOS-CG-2021: A Mixture Model for the Calculation of Thermodynamic Properties of CCS Mixtures.
Int. J. Thermophysics (2023), 44. https://doi.org/10.1007/s10765-023-03263-6

SWAN Analytische Instrumente AG, Hinwil (Switzerland)

Mar Nogales

Following Technical Guidance Document (TGD) is presently in revision:

- TGD2-09(2015) Instrumentation for monitoring and control of cycle chemistry for the steam-water circuits of fossil-fired and combined cycle power plants

During 2023 and 2024, this TGD will be reviewed. Based on this, the document is updated/revised.

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. Results of the common work concerning the modification of the van der Waals and Platteeuw model in order to consider multiple cage occupancy for hydrogen hydrates have been published in a joint publication at the beginning of this year [1].
2. Within the project “Optisyskom”, heat transfer coefficients in annular cavities in the casing of steam turbines are investigated experimentally and theoretically. The first experimental campaign with air is finished and the results have been presented and published at the AG Turbo Statusseminar in Cologne [2].

Recent Publications:

[1] Fiedler, F.; Vinš, V.; Jäger, A.; Span, R.:
Modification of the van der Waals and Platteeuw Model for Gas Hydrates Considering Multiple Cage Occupancy.
Journal of Chemical Physics (2024), 160 (9), 094502.
https://doi.org/10.1063/5.0189555.

[2] Paulick, O.; Jäger, A.; Eschmann, G.; Uffrecht, W.; Worlitz, N.:
Thermofluiddynamik in Gehäuseseitenräumen mit Dampfzufuhr und -entnahme im lastflexiblen Betrieb von Industriedampfturbinen.
In Tagungsband 18. Statusseminar AG Turbo; Cologne (2024).

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

Projects

1. 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.
2. 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).
   - Implementation and verification in the software KRAWAL of Siemens
3. Application of the Spline-Based Table Look-Up Method (SBTL) to ammonia-water mixtures
   - SBTL functions have been developed for the vapor-liquid phase equilibrium of ammonia-water mixtures. The phase equilibrium is calculable from (p,T), (p,ξ_l), (p,ξ_v), (T,ξ_l), and (T,ξ_v) inputs. These functions guarantee convergence and drastically increase the computing speed.
   - Three dimensional SBTL functions are being developed in order to demonstrate the method for three independent input variables as in $T(p,h,\xi)$.
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 from the IAPWS Formulation 2011 for the thermal conductivity of water are being incorporated into the 2025 ASHRAE Handbook of Fundamentals.

Recent Publications

- Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Wagner, W.; Friend, D. G.; Harvey, A. H.:
  Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL).
  J. Eng. Gas Turbines Power, in preparation.
- Herrmann, S.; Vogel, E.:
  Viscosity Measurements on Natural Gas: Re-evaluation.
  Int. J. Thermophys. 44, 177 (2023).
  https://doi.org/10.1007/s10765-023-03280-5

Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, June, 2024

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

I. Overview:

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

II. Recent Publications:

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

Novel approach for designing order parameters of clathrate hydrate structures by graph neural network
S. Ishiai, K. Endo, P. E. Brumby, A. K. Sum, K. Yasuoka
J. Chem. Phys., 160, 064504 (11 pages), 2024

Graph-Neural-Network-Based Unsupervised Learning of the Temporal Similarity of Structural Features Observed in Molecular Dynamics Simulations
S. Ishiai, I. Yasuda, K. Endo, K. Yasuoka
J. Chem. Theory Comput., 20, 819-831, 2024

Unsupervised deep learning for molecular dynamics simulations: a novel analysis of protein–ligand interactions in SARS-CoV-2 Mpro
J. Mustali, I. Yasuda, Y. Hirano, K. Yasuoka, A. Gautieri, N. Arai
RSC Adv., 13, 34249-34261, 2023

Pre-Smectic Ordering and the Unwinding Helix in Monte Carlo Simulations of Cholesteric Liquid-Crystals
P. E. Brumby, A. Kowaguchi, T. Nozawa, K. Yasuoka, H. Wensink
J. Phys. Chem. B, 127, 7194-7204, 2023

Graph neural networks classify molecular geometry and design novel order parameters of crystal and liquid
S. Ishiai, K. Endo, K. Yasuoka
J. Chem. Phys., 159, 064103 (16 pages), 2023

Report on IAPWS Annual Meeting 2022
K. Yoshida, K. Yasuoka
The Thermal and Nuclear Power, 74, 46-52, 2023

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., 8, 652-661, 2023

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, 15, 8567-8578, 2023

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

Solvation dynamics on the diffusion timescale elucidated using energy-represented dynamics theory
K. Okita, N. Ito, N. Morishita-Watanabe, H. Umakoshi, K. Kasahara, N. Matubayasi
Phys. Chem. Chem. Phys., 26, 12852-12861, 2024

How ATP suppresses the fibrillation of amyloid peptides: analysis of the free-energy contributions
T. M. Do, D. Horinek, N. Matubayasi
Phys. Chem. Chem. Phys., 26, 11880-11892, 2024

Biased Bowl-Direction of Monofluorosumanene in the Solid State
Y. Yakiyama, M. Li, D. Zhou, T. Abe, C. Sato, K. Sambe, T. Akutagawa, T. Matsumura, N. Matubayasi, H. Sakurai
J. Am. Chem. Soc., 146, 5224-5231, 2024

Actual Amount Adsorbed as Estimated from the Surface Excess Isotherm
S. Shimizu, N. Matubayasi
Langmuir, 40, 1666-1673, 2024

Free-energy decomposition of salt effects on the solubilities of small molecules and the role of excluded-volume effects,

S. Hervø-Hansen, D. Lin, K. Kasahara, N. Matubayasi
Chem. Sci., 15, 477-489, 2024

Replacing the Langmuir Isotherm with the Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
J. Phys. Chem. Lett., 15, 3683-3689, 2024

Unraveling the Glass-like Dynamic Heterogeneity in Ring Polymer Melts: From Semiflexible to Stiff Chain
S. Goto, K. Kim, N. Matubayasi
ACS Polym. Au, 3, 437-446, 2023

Elucidating protein-ligand binding kinetics based on returning probability theory
K. Kasahara, R. Masayama, K. Okita, N. Matubayasi
J. Chem. Phys., 159, 134103 (15 pages), 2023

Cooperativity in Sorption Isotherms
S. Shimizu, N. Matubayasi
Langmuir, 39, 13820-13829, 2023

Molecular Dynamics Study of the Antifouling Mechanism of Hydrophilic Polymer Brushes
T. Yagasaki, N. Matubayasi
Langmuir, 39, 13158-13168, 2023

Sorption from Solution: A Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
Langmuir, 39, 12987-12998, 2023

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,
J. Chem. Phys., 158, 174901 (10 pages), 2023

Arylazopyrazole-Based Photoswitchable Inhibitors Selective for *Escherichia coli* Dihydrofolate Reductase
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

Hyper-mobile Water and Raman 2900 cm^{-1} Peak Band of Water Observed around Backbone Phosphates of Double Stranded DNA by High-Resolution Spectroscopies and MD Structural Feature Analysis of Water

M. Suzuki, A. Tsuchiko, Y. Tanaka, N. Matubayasi, G. Mogami, N. Uozumi, S. Takahashi,
J. Phys. Chem. B, 127, 285-299, 2023
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

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

Effect of Cage Occupancies on Molecular Vibrations of Methane in Structure H Clathrate Hydrate: Ab Initio Molecular Dynamics Simulation
K. Yoshida, S. Suhara, N. Noguchi
J. Phys. Chem. B, 2024, DOI: 10.1021/acs.jpcb.4c01790

Report on IAPWS Annual Meeting 2022
K. Yoshida, K. Yasuoka
The Thermal and Nuclear Power, 74, 46-52, 2023

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

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

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

Uchida, Hiroshi
Senior Researcher, Physical and Chemical Oceanography Research Group, Global Ocean Observation Research Center, Research Institute for Global Change, Japan Agency for Marine-Earth Science and Technology (JAMSTEC)
Email: huchida@jamstec.go.jp

Turbulence across the Antarctic Circumpolar Current in the Indian Southern Ocean: Micro-temperature measurements and finescale parameterizations
Y. Sasaki, I. Yasuda, K. Katsumata, S. Kouketsu, H. Uchida
J. Geophys., Res.: Oceans, 129, e2023JC019847, 2024

Simple design method for ceramic tube pressure housings

Y. Maeda, T. Aso, H. Uchida
IEEE J. Oceanic Engineering, in press, 2024

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

Biogas separation by semiclathrate hydrates formed with tetra-*n*-butylammonium and tetra-*n*-butylphosphonium salts
S. Muromachi, K. Ikeda, K. Maesaka, H. Miyamoto
Energy, 290, 130176 (9 pages), 2023

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

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

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., 39(8), 1361-1370, 2023

Ichihara, Taro
Senior Engineer, Plant Service Division, Mitsubishi Heavy Industries Power IDS, Ltd.
Email: taro.ichihara.jp@mhi.com

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)

Nakatsuchi, Yuta
Deputy Manager, Research & Innovation Center, Mitsubishi Heavy Industries, Ltd.
Email: yuta.nakatsuchi.mc@mhi.com

Study of Novel Water Quality Management System in the Steam-Water Circuit of Gas Turbine Combined Cycle Power Plants

Y. Nakatsuchi
Osaka University, Ph. D. thesis, 2024 (in Japanese)

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, 56, 2238770, 2023

Ishihara, Nobuo
Engineering Manager, Nuclear Energy Segment, Mitsubishi Heavy Industries, Ltd.
Email: nobuo.ishihara.2x@nu.mhi.com

Big Data Factorial Analysis using Plant Operational Data for Dose Rate Reduction
N. Ishihara, Y. Mukai, S. Yamazaki, A. Maeda
NPC 2023 – International Conference on Water Chemistry in Nuclear Reactor Systems, France, Juan-les-Pins, 2023

III. Presentations at JPAPWS General Meetings:

FY2024 1st General Meeting, May 28, 2024
Development of Novel Water Quality Management method for Water-Steam Circuits of Gas Turbine Combined Cycle Power Plants
Yuta Nakatsuchi（Mitsubishi Heavy Industries, Ltd.）

Adsorption Behavior of OLDA and the Effect of Adsorbed OLDA on Contact Angle
Yuta Nakatsuchi（Mitsubishi Heavy Industries, Ltd.）

Cage Occupancy Analysis and Phase Diagram Prediction in Clathrate Hydrates through Monte Carlo Simulations
Hirotaka Kishimoto（Keio University）

FY2023 5th General Meeting, March 11, 2024
Energy Process Research Institute (EPRI), National Institute of Advanced Industrial Science and Technology
Sanehiro Muromachi（AIST）

Revealing the hidden dynamics of confined water in acrylate polymers: Insights from hydrogen-bond lifetime analysis
Kokoro Shikata（Osaka University）

FY2023 4th General Meeting, January 30, 2024
Retro-technology, Electric Thermal Energy Storage realizes economic de-carbonized society
Toru Okazaki（The Institute of Applied Energy）

Molecular dynamics study on the surface structure of alcohol-water mixture
Mayu Hirose（University of Toyama）, Tatsuya Ishiyama（University of Toyama）

FY2023 3rd General Meeting, December 7, 2023

Hydrogen damage in a power boiler - Correlations between damage distribution and thermal-hydraulic properties
Taro Ichihara (Mitsubishi Heavy Industries Power IDS, Ltd.)

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)

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)

U.S. National Committee to IAPWS
2024 Report on Activities of Potential Interest to IAPWS

Communicated from the National Institute of Standards and Technology, Boulder, CO and Gaithersburg, MD:

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 (and heavy water). This includes the electronic and vibrational polarizabilities, the dipole moment, and the rotational quantum effects that cause the dielectric constant to deviate from the classical Debye expression. The work has been published: G. Garberoglio, C. Lissoni, L. Spagnoli, and A.H. Harvey, "Comprehensive quantum calculation of the first dielectric virial coefficient of water," *J. Chem. Phys.* **160**, 024309 (2024). This work will provide boundary conditions for future IAPWS formulations for the dielectric constant of water and of heavy water, and can support proposed capacitance-based measurements for humidity.

High-accuracy refractivity measurements have been performed on water vapor (and heavy water vapor) between 293 K and 433 K at an optical frequency, and at 303 K at a frequency in the near infrared. Comparison with the IAPWS formulation for the refractive index of ordinary water indicates that there is some room for improvement, with about a 2% discrepancy in the low-density limit. References: P.F. Egan and Y. Yang, "Optical $n(p, T_{90})$ measurement suite 2: H_2O and D_2O," *Int. J. Thermophys.* **45**, 89 (2024); P.F. Egan and Y. Yang, "Optical $n(p, T_{90})$ measurement suite 3: Results at $\lambda = 1542$ nm," *Int. J. Thermophys.*, in preparation.

Communicated from OLI Systems Inc., Parsippany, NJ:

Aqueous chemistry of critical materials

OLI Systems continued its participation in the Department of Energy's Critical Materials Innovation Hub (CMI). OLI's work focuses on developing thermodynamic models for predicting chemical and phase equilibria in systems containing rare earth elements, nickel, cobalt, lithium, and other critical materials. In the past year, the work was focused on (1) developing thermodynamic models for rare earth carbonates, fluorocarbonates, oxyfluorides, and oxychlorides, (2) finalizing a model for optimizing the recovery of metals from end-of-life lithium ion battery cathodes using gluconic acid as an environmentally benign, biologically-sourced lixiviant, (3) finalizing a model for the crystallization of cobalt and nickel in the form of Tutton salt crystals, (4) studying the recovery of cadmium and tellurium from end-of-life solar panels and (5) initiating research on modeling solvent extraction of rare earths. The results of project (2) have been published in the following paper:

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," *Resources, Conservation & Recycling* **199** (2023) 107293.

Modeling aqueous nuclear power chemistry

OLI has completed a collaborative project with the University of Guelph on developing a comprehensive model for the behavior of aqueous systems containing boric acid and borates of lithium, sodium, and potassium. The work was based on the recent experimental results from the

University of Guelph, which elucidated speciation of borates at high temperatures. The work has been published in the following paper:

P. Wang, A. Anderko, and P. Tremaine, "Speciation and phase equilibria of aqueous boric acid and alkali metal borates from ambient to hydrothermal conditions: a comprehensive thermodynamic model," *Ind. Eng. Chem. Res.* **62** (2023) 20875–20898