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

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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