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

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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.