German National Committee to IAPWS Executive Committee

Research Activities on the Thermodynamic Properties of Water and Steam of the German National Committee and of Partners in Switzerland in the Period 2020/2021

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

Vice Chair: Ingo Weber
Spardorf

Annual Meeting of the German National Committee

The Annual Meeting of the German National Committee was planned at the GFZ German Research Centre for Geosciences in Potsdam for March 2021, but had to be canceled due to Corona situation.

In the following, activities of certain members of the German National Committee are summarized.

Baltic Sea Research Institute, Warnemuende
Dr. Rainer Feistel

Recent Publications

- Ebeling, W., Feistel, R., Camoes, M.F.:
  Trends in statistical calculations of individual ionic activity coefficients of aqueous electrolytes and seawater.
  Trends in Physical Chemistry (2020), 20:1-26
  http://www.researchtrends.net/tia/abstract.asp?in=0&vn=20&tid=16&aid=6609&pub=2020&type=3
- Weinreben, S., Feistel, R.:
  Anomalous salinity-density relations of seawater in the eastern central Atlantic.
  Deep–Sea Research I 154 (2019) 103160, https://doi.org/10.1016/j.dsr.2019.103160
- Feistel, R.:
  Distinguishing between Clausius, Boltzmann and Pauling Entropies of Frozen Non-equilibrium States.
  Entropy 2019, 21(8), 799; https://doi.org/10.3390/e21080799
  (Editor's Choice article)
- Hellmuth, O., Schmelzer, J.W.P., Feistel, R.:
  Ice-Crystal Nucleation in Water: Thermodynamic Driving Force and Surface Tension. Part I: Theoretical Foundation.
  Entropy 2020, 22(1), 50; https://doi.org/10.3390/e22010050
- Feistel, R., Hellmuth, O.:
  Zur Rolle des Wassers in der Energiebilanz des Klimasystems.
  Sitzungsberichte der Leibniz-Sozietät der Wissenschaften zu Berlin 144 (2020) 51-139,
  https://leibnizsozietaet.de/publikationen/sitzungsberichte/

English translation:
On the Role of Water in the Energy Balance of the Climate System,
https://doi.org/10.13140/RG.2.2.19649.17766

- Hellmuth, O., Feistel, R.:
  Analytical Determination of the Nucleation-Prone, Low-Density Fraction of Subcooled Water.
  Entropy 2020, 22(9), 933; https://doi.org/10.3390/e22090933
- Ebeling, W.; Feistel, R.; Krienke, H.:
  On statistical calculations of individual ionic activity coefficients of electrolytes and seawater. I.
  Online preprint 14 Apr 2019.
  DOI: 10.13140/RG.2.2.18591.20640
- Feistel, R.:
  Defining relative humidity in terms of water activity. Part 2: relations to osmotic pressures.
  Metrologia 56, 015015 (2019).
  https://doi.org/10.1088/1681-7575/aaf446
- Hellmuth, O.; Shchekin, A. K.; Feistel, R.; Schmelzer, J. W. P.; Abyzov, A. S.:
  Physical interpretation of ice contact angles, fitted to experimental data on immersion freezing of kaolinite particles.
  Interface. Phenom. Heat Transfer 6, 37-74 (2018).
  DOI: 10.1615/InterfacPhenomHeatTransfer.2018026166
- Hellmuth, O., Feistel, R.; Foken, T.:
  Intercomparison of Different State-of-the-Art Formulations of the Mass Density of Humid Air.
  Bull. Atmos. Sci. Tech. (2021), in press, https://doi.org/10.1007/s42865-021-00036-7
- Feistel, R.:
  Thermodynamic Properties of Seawater, Ice and Humid Air: TEOS-10, Before and Beyond.
  Ocean Sci. 14, 471-502 (2018).
  https://doi.org/10.5194/os-14-471-2018
- Burchard, H.; Bolding, K.; Feistel, R.; Gräwe, U.; Klingbeil, K.; MacCready, P.; Mohrholz, V.; Umlauf, L.; van der Lee, E.:
  The Knudsen theorem and the Total Exchange Flow analysis framework applied to the Baltic Sea.
  Progress in Oceanography 165, 268-286 (2018).
  https://doi.org/10.1016/j.pocean.2018.04.004
- Feistel, R.; Lovell-Smith, J. W.:
  Implementing systematic error in the weight matrix of generalized least-squares regression.
  published online (2018).
  https://doi.org/10.13140/RG.2.2.25098.16320

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

Projects

1. Thermophysical properties of mixtures of water vapor and simple gases from first-principles calculations.
2. Measurements of the speed of sound in water and derived thermodynamic properties of water.

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.
  N.N. (2021), in preparation.

Leibniz Institute for Tropospheric Research, Leipzig
Dr. Olaf Hellmuth

Recent Publications (published, in press, submitted, in preparation)

- 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 (book chapter). In press.
- Görner, C.; Franke, J.; Kronenberg, R.; Hellmuth, O.; Bernhofer, C.:
  Multivariate non-parametric Euclidean distance model for hourly disaggregation of daily climate data.
  Theoretical and Applied Climatology, 143, pp. 241-265, https://doi.org/10.1007/s00704-020-03426-7 (journal article).
- Hellmuth, O.; Feistel, R.; Foken, T.:
  Intercomparison of different state-of-the-art formulations of the mass density of humid air.
  Bulletin of Atmospheric Science and Technology.
  Bull. Atmos. Sci. Tech. doi:10.1007/s42865-021-00036-7 (journal article).
- 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, in (book chapter). In press.
- Spänkuch, D., O. Hellmuth, U. Görsdorf: What is a cloud? Toward a more precise definition? Bull. Am. Met. Soc. (journal article). In Revision
- Feistel, R., F., Hellmuth, O.:
  Zur Rolle des Wassers in der Energiebilanz des Klimasystems. In: Pfaff, G., R. O. Greiling, R. Pail: Klimawandel – Anzeichen, Ursachen, Folgen.
  Kolloquium der Leibniz-Sozietät der Wissenschaften zu Berlin am 13.2.2020 in der Humboldt-Universität Berlin. Sitzungsberichte der Leibniz-Sozietät der Wissenschaften, Band 144, 51-139, https://leibnizsozietaet.de/wp-content/uploads/2021/03/Gesamtdatei-SB-144-2020.pdf (book chapter).
- Feistel, R., F., Hellmuth, O.:
  On the Role of Water in the Energy Balance of the Climate System.
  Vortrag am 13. Feb. 2020, Kolloquium „Klimawandel – Anzeichen, Ursachen, Folgen“.
  Leibniz-Sozietät der Wissenschaften zu Berlin e.V., ResearchGate, https://doi.org/10.13140/RG.2.2.36390.88649 (conference contribution).

- Hellmuth, O., Feistel, R.:
  Analytical determination of the nucleation-prone, low-density fraction of subcooled water.
  Entropy 2020, 22(9), 933, https://doi.org/10.3390/e22090933 (journal article)

PPCHEM AG, Hinwil - Switzerland
Michael Rziha

Following Documents are presently in elaboration:

- 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
- Chemistry for Electrode Boilers (White Paper)
- FFS application in Nuclear Plants (White paper)
- Demin Water Integrity
- Condensate Polishing Plants
- Smart Alarms

Due to the well-known pandemic situation in 2020 and 2021 the progress of these documents was hampered.

Nevertheless, several documents were progressing well, while some others did not progress for different reasons at all.

Based on this individual status, initial feedback from the PCC WG and the progress forecast it was decided by PCC to divide the individual documents, respectively its status into 3 groups, namely:

- Active
- Static - Retired
- New

Consequently, it was jointly agreed to "retire" the TGD "Demin. Water Integrity", as there was no significant progress during the last 5 years.

The elaboration of the TGD "Smart Alarms" became also retired, since several aspects (e. g. legal issues, as the term "Smart Alarms" is licensed by EPRI) are clearly speaking against such an individual TGD. It was jointly agreed to prepare an amendment to the existing IAPWS TGD2-09(2015) "Instrumentation", covering this topic accordingly and in an appropriate manner.

TGD Condensate Polishing Plants will be kept alive until 2022. In case of there is no significant progress visible until 2022, its retirement will be likely and will be decided during the annual meeting in 2022.

All other documents, as listed here before, will remain active.

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

Projects:

1. The working group 3.13 'Electrochemistry' of PTB 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, working group 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. PTB 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.

PTB German National Metrology Institute
Working Group 7.42, Applied Thermometry
Dr. Steffen Rudtsch

Projects:

1. Measurements of the speed of sound in water, heavy water and seawater.

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 Shar-C for high-fidelity, scale-resolving calculations of unsteady, turbulent, condensing wet steam flows in low-pressure turbines.
    - The in-house, density-based CFD solver Shar-C 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) and combustion.
    - At current times, wet steam flows are treated by means of the mono-dispersed Source-Term Euler-Euler model and the non-equilibrium condensation effects are modeled based on the classical theory of droplet nucleation and droplet growth.
    - A considerable computational speed is obtained, where the SBTL method shows an overhead of only 2% compared to a baseline ideal gas computation; a full condensation computation is only connected to an overhead of 26%.
    - For high quality LES computations, the solver is equipped with a hybrid, low-dissipation spatial discretization scheme for accurate treatment of turbulence in presence of shock waves and discontinuities due to condensation.
    - The first large eddy simulation of a realistic condensing wet steam flow was presented in 2020: Overall, the LES results are much better able to reproduce the experimental data compared to standard RANS and URANS computations. Based on the SBTL and a highly-optimized code, the LES on a grid with 48 million cells could be conducted in a computational time of 1000 CPU weeks.
2. Implementation of extensions of the SBTL method to humid air and other flow media like CO2 into the in-house code Shar-C.
3. Implementation of the SBTL method into an in-house high-order finite-difference code targeted towards direct numerical simulations of compressible real gas flows for computations on GPUs.
4. Implementation of a new unstructured FVM and high-order DG solver for the solution of complex thermodynamic flows (like condensing wet steam flows) in complex geometries and for scale-resolving computations.
5. Investigation the use of Physics Informed Artificial Neural Networks for the Physics Recovery to advance the state of condensation Modeling.

Recent Publications

- Post, P.; Winhart, B.; di Mare, F.:
  Large Eddy Simulation of a Condensing Wet Steam Turbine Cascade.
  J. Eng. Gas Turbines Power, GTP-20-1526.
- Post, P.; Winhart, B.; di Mare, F.:
  Large Eddy Simulation of a Condensing Wet Steam Turbine Cascade.
  ASME Paper GT2020-16064, Proceedings of ASME Turbo Expo 2020: Turbine Technical Conference and Exposition GT2020, London, UK.
- Karaefe, E. K.; Post, P.; Sembritzky, M.; Schramm, A.; Kunick, M.; Gampe, U.; di Mare, F.:
  Numerical Investigation of a Centrifugal Compressor for Supercritical CO2 Cycles.
  ASME Paper GT2020-15194, Proceedings of ASME Turbo Expo 2020: Turbine Technical Conference and Exposition GT2020, London, UK.

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

Projects:

- Our project on hydrate formation, 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 reached its (preliminary) end. With the defense of the thesis of Dr. Sebastian Hielscher the active work ended. Results were published in Journals [1,2] and on national and international conferences. A follow up proposal has been submitted to the German Science Foundation (DFG), involving Dr. V. Vins as “Mercator Fellow”. A decision regarding the proposal is expected by the end of 2021.
- Our work on consideration of salts in water and in mixtures containing water is progressing. It has been shown that the IAPWS seawater equation can be used in Helmholtz-energy based mixture models. This way mixtures with brines can be described using the framework of equations of state established for natural gases and CO_2-rich mixtures. Results were presented on national and international conferences, were presented to IAPWS TPWS by Benedikt Semrau, and were submitted to an international journal [3]. However, the use of the IAPWS seawater model results in restrictions regarding allowable salt composition, salinity and temperature and pressure range. To come to a more general description of brines, the model is currently extended using a Pitzer approach to describe the electrolytes. First results were presented were presented on national and international conferences, and to IAPWS TPWS. The project received funding by the EU / ERA ACT project ELEGANCY and by the Fraunhofer high performance center DYNAFLEX. Currently funding for continued work is missing.

- In particular for CCS application aqueous mixtures with amines are relevant, be it for capture processes, where high amine concentrations are typical, or for transport, where water and amines are minor components in CO_2-rich mixtures. A physically sound description of these mixtures requires models that are able to represent the behavior of reacting systems. Typically, these models are excess Gibbs-enthalpy models (g^E models), which are able to describe phase equilibria relatively well, but which do not describe properties of homogeneous states and of coexisting phases well. A project carried out in cooperation with a colleague at the NTNU in Trondheim (Prof. Jana Poplsteinova Jakobsen) aims at the implementation of a g^E model into a Helmholtz mixture model to combine the description of VLE of reacting mixtures with the accuracy of Helmholtz mixture models for the description of thermodynamic properties.

First results are promising and have been presented on national and international conferences by Tobias Neumann; a journal publication is under preparation. The project received funding by the Norwegian CCS Center (NCCS) led by SINTEF Energy. Currently funding for continued work is missing.

[1] *S. Hielscher, V. Vinš, A. Jäger, J. Hrubý, C. Breitkopf, and R. Span:* A new approach to model mixed hydrates. In: Fluid Phase Equilibria 459, 170-185 (2018).
[2] *S. Hielscher, B. Semrau, A. Jäger, V. Vinš, C. Breitkopf, J. Hrubý, and R. Span:* Modification of a model for mixed hydrates to represent double cage occupancy. Fluid Phase Equilibria 490, 48-60 (2019).
[3] *B. Semrau, S. Hielscher, M. Thol, and R. Span:* Combination of Gibbs and Helmholtz energy equations of state in a multiparameter mixture model using the IAPWS seawater model as an example. Submitted to Int. J. Thermophysics (2021).

Technical University of Dresden
Institute of Power Engineering, Chair of Technical Thermodynamics
Prof. Dr. Cornelia Breitkopf, Dr. Andreas Jäger

Projects:

- Development of an algorithm for fitting the model parameters of the combination of the multi-fluid mixture model with the excess Gibbs energy models UNIFAC and COSMO-SAC. In a first step, the algorithm will be applied for fitting water + linear alkane mixtures with the focus on Henry coefficients for these mixtures.

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

Projects

1. 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 ASHRAE Standard, Method for Calculating Moist Air Thermodynamic Properties.
2. Preparation of Chapter 1 Psychrometrics for the 2021 ASHRAE Handbook of Fundamentals. The equations for thermodynamic properties of the IAPWS-IF97 Industrial Formulation and the equations for transport properties of the IAPWS Formulation 2008 for the viscosity and the IAPWS Formulation 2011 for the thermal conductivity of water have been incorporated into the 2021 ASHRAE Handbook of Fundamentals.

Recent Publications

- 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.

Zittau/Goerlitz University of Applied Sciences
Faculty of Mechanical Engineering, Dept. of Energy Systems Technology, Zittau
Prof. Dr. Matthias Kunick

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).

Recent Publications

- Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.; Friend, D. G.; Harvey, A. H.:
  Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL).
  J. Eng. Gas Turbines Power, in preparation.