German National Committee to IAPWS Executive Committee

Research Activities on the Thermodynamic Properties of Water and Steam of the German National Committee in the Period 2019/2020

www.iapws.de

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

Vice Chair: Ingo Weber
Siemens Power and Gas, Erlangen

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 27th, 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), in press
- 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 zu Berlin, im Druck
- 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.
  Interfac. Phenom. Heat Transfer 6, 37-74 (2018).
  DOI: 10.1615/InterfacPhenomHeatTransfer.2018026166
- Hellmuth, O.; Feistel, R.; Foken, T.:
  Technical Note: Intercomparison of Different State-of-the-Art Formulations of the Mass Density of Humid Air.
  Atmos. Chem. Phys. (2020), to be submitted.
- 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.:
  Reference Values for the Cross Second Virial Coefficients and Dilute Gas Binary Diffusion Coefficients of the Systems ($H_2O + O_2$) and (H_2O + Air) from First Principles.
  J. Chem. Eng. Data 65, 4130-4141 (2020).
- Hellmann, R.; Harvey, A. H.:
  First-Principles Diffusivity Ratios for Kinetic Isotope Fractionation of Water in Air
  Geophys. Res. Lett. (2020), DOI: 10.1029/2020GL089999.
- 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. (2020), in preparation.

Leibniz Institute for Tropospheric Research, Leipzig
Dr. Olaf Hellmuth

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

- Feistel, R., F., Hellmuth, O.:
  Zur Rolle des Wassers in der Energiebilanz des Klimasystems. Sitzungsberichte der Leibniz-Sozietät der Wissenschaften zu Berlin, 144 (2020). In press.
- Feistel, R., F., Hellmuth, O.:
  On the Role of Water in the Energy Balance of the Climate System. (English translation of the German article „Zur Rolle des Wassers in der Energiebilanz des Klimasystems“, Sitzungsberichte der Leibniz-Sozietät der Wissenschaften 144 (2020).
- Foken, T.; Hellmuth, O.; Huwe, B.; Sonntag, D.:
  Chapter 6: Physical Quantities. In: T. Foken (ed.): Springer Handbook of Atmospheric Measurements. Springer. In press (to be published in 2021).
- Sonntag, D.; Foken, T.; Vömel, H.; Hellmuth, O.:
  Chapter 9: Humidity Sensors. In: T. Foken (ed.): Springer Handbook of Atmospheric Measurements. Springer. In press (to be published in 2021).
- Görner, Ch.; Franke, J.; Kronenberg, R.; Hellmuth, O.; Bernhofer, Ch.:
  Multivariate non-parametric Euclidean distance model for hourly disaggregation of daily climate data. Theoretical and Applied Climatology, submitted (under revision).
- Hellmuth, O., Feistel, R., 2020: Analytical determination of the nucleation-prone, low-density fraction of subcooled water. Entropy 2020, 22, 993, doi:10.33909/e22090933 (2020).
- 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. Submitted (2020).
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Real-Gas Effects in Humid Air: Possible Implications of the Advanced Seawater Standard TEOS-10 for Hygrometry at Atmospheric Pressure.
  Part I: Thermostatic Foundation.
  Part II: Performance of Enhancement Factor and Relative Fugacity. Wiss. Mitteil. Inst. f. Meteorol. Univ. Leipzig. In preparation.
- Hellmuth, O.; Feistel, R.:
  Real-Gas Effects in Humid Air: Possible Implications of the Advanced Seawater Standard TEOS-10 for Hygrometry at Atmospheric Pressure. Part III: Effects on Radiative Warming and Cooling in the Water-Vapour Absorption Bands and on the Surface Energy Balance.
  Wiss. Mitteil. Inst. F. Meteorol. Univ. Leipzig. In preparation.
- Hellmuth, O.; Schmelzer, J. W. P.; Feistel, R.:
  Ice-crystal nucleation in water: Thermodynamic driving force and surface tension. Part I: theoretical foundation. Entropy, 22, 50, doi:10.3390/e22010050 (2020).
- Hellmuth, O., Schmelzer, J. W. P., Feistel, R.:
  Ice-crystal nucleation in water: Thermodynamic driving force and surface tension. Part II: verification. In preparation.

PPCHEM AG, Hinwil - Switzerland
Michael Rziha (Germany)

Activities

- New TGD on Air In Leakage (AIL) released and available at the IAPWS homepage
- New TGD on film forming substances (FFS) for industrial plants released and available at the IAPWS homepage.
- New TGD Chemistry Management in Generator Water Cooling during Operation and Shutdown released and available at the IAPWS homepage

- Revision of TGD8-16 on Application of FFS in Fossil, Combined Cycle and Biomass Plants released and available at the IAPWS homepage
- Ongoing writing of the white paper about FFS application in nuclear plants
- Finalization of the white paper on corrosion product monitoring in flexible (cycling and two-shifting) plants
- Preparation of the new TGD on Flue Gas Condensation and it`s re-use

The elaboration of the white paper on chemistry for geothermal plants is in further progress.

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

Project:

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.

Recent Publications

- Post, P.; Winhart, B.; di Mare, F.:
  Large Eddy Simulation of a Condensing Wet Steam Turbine Cascade.
  J. Eng. Gas Turbines Power, in preparation.
- 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.

- Post, P.; Sembritzky, M.; di Mare, F.:
  Towards scale resolving computations of condensing wet steam flows.
  ASME Paper GT2019-91269, Proceedings of ASME Turbo Expo 2019: Turbine Technical Conference and Exposition GT2019, June 17 – 21, 2019, Phoenix, Arizona, USA.
- Iseni, S.; Post, P.; Sembritzky, M.; di Mare, F.:
  Numerical analysis of the influence of air humidity on a transonic compressor stage.
  Proceedings of the IGTC 2019 Conference, 17th-22nd November, 2019, Tokyo, Japan.
- Post, P.; Winhart, B.; di Mare, F.:
  Large eddy simulation of a condensing flow in a steam turbine cascade.
  Proceedings of the IGTC 2019 Conference, 17th-22nd November, 2019, Tokyo, Japan.
- 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.

Siemens Power and Gas, Erlangen
Ingo Weber

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.

STEAG Energy Services, Zwingenberg
Dr. Reiner Pawellek, Dr. Tobias Löw

Project

1. Preparation of a fast IAPWS-IF97 property library using SBTL algorithms iteration start values for backward functions.

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.

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

Projects:

1. The work on the combination of the multi-fluid mixture model with excess Gibbs energy models, especially the predictive model COSMO-SAC, continues. Recently we published an open-source implementation of three different COSMO-SAC models comprising a database of sigma-profiles for about 2262 components including water.

Recent Publications

- Bell, I.H.; Mickoleit, E.; Hsieh, C.-M.; Lin, S.-T.; Vrabec, J.; Breitkopf, C.; Jäger, A. (2020): A Benchmark Open-Source Implementation of COSMO-SAC, J. Chem. Theory Comput. 16(4), 2635–2646.

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

Projects

1. Development of fast property calculation algorithms based on spline interpolation
   - The Spline-Based Table Look-Up Method (SBTL) is being applied to the mixture humid air.
2. Application of the developed SBTL method for calculating thermodynamic properties

   The developed spline-based property libraries have been implemented into the following process simulation codes:
   - Non-stationary thermo-hydraulic code ATHLET of the German Society of Global Research for Safety (GRS), Garching
   - Non-stationary thermo-hydraulic code RELAP-7 of the Idaho National Laboratory (INL)
   - Process simulation software of Fraunhofer UMSICHT, Oberhausen
3. Development of a new ASHRAE standard for calculating thermodynamic properties of moist air, ASHRAE Project SPC-213P.
4. Preparation of Chapter 1 for the 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.; 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.
- 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, in preparation.