Research Activities on the Thermodynamic Properties of Water and Steam of the German National Committee in the Period 2017/2018

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Chair: Ingo Weber, Siemens Power and Gas, Erlangen

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

Annual Meeting of the German National Committee

The 2018 Annual Meeting of the German National Committee took place at the Leibniz Institute for Tropospheric Research in Leipzig on 9th March 2018. 23 Colleagues attended this meeting. Six papers were presented in the scientific session.

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

Baltic Sea Research Institute, Warnemuende
Dr. Rainer Feistel

Recent Publications
- 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.
  Volume 165, July–August 2018, Pages 268-286 (2018).
  https://doi.org/10.1016/j.pocean.2018.04.004, in press
- 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
- Hellmuth, O.; Shchekin, A.K.; Feistel, R.; Schmelzer, J.W.P.; Abyzov, A.S.:
  Physical Interpretation of Ice Contact Angels, Fitted to Experimental Data on Immersion Freezing of Kaolinite Particles.
  Interfacial Phenomena and Heat Transfer, 2017 (in press).
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.
  N.N. (2018), in preparation.
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
  Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air".
  N.N. (2018), in preparation.

Baltic Sea Research Institute, Warnemuende
Dr. Stefan Weinreben

Projects

1. Measurements of density and practical salinity in the Baltic Sea to determine the absolute salinity anomaly

2. Preparation of a paper about measurements of the density-anomaly in the Atlantic Ocean.

3. We got the ILAC-accreditation for the calibration laboratory of the IOW for the calibration of oceanographic devices for electrical conductivity, temperature and pressure.

German Aerospace Center (DLR), Cologne
Institute of Propulsion Technology
Prof. Dr. Francesca di Mare

Project

1. Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the CFD Code TRACE.
   o The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the CFD code TRACE.
   o On this basis the implementation has been further improved, especially regarding the software architecture, solution algorithm and boundary treatment.
   o The capability of the SBTL-method has been tested on Laval-nozzle and Cascade test cases. The calculation of a real steam engine configuration is targeted next.

Recent Publications
   o 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.

Leibniz Institute for Tropospheric Research, Leipzig
Dr. Olaf Hellmuth

Projects

1. Preparation of a Paper about Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air

2. Preparation of Three Further Volumes on New Particle Formation in the Earth Atmosphere

Recent Publications
   o Hellmuth, O.; Shchekin, A.K.; Feistel, R.; Schmelzer, J.W.P.; Abyzov, A.S.:
   Physical Interpretation of Ice Contact Angels, Fitted to Experimental Data on Immersion Freezing of Kaolinite Particles.
   Interfacial Phenomena and Heat Transfer, 2017 (in press).

   o Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
   Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.
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o Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.:
Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air".
N.N. (2018), in preparation.

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

Projects:

1. Development of a new reference equation of state for heavy water. This work is linked to an IAPWS grant awarded in 2012 and to a close cooperation with Dr. A. H. Harvey and Dr. E. W. Lemmon at NIST in Boulder, CO. The work on the new equation of state has largely been finished. A draft release will be submitted to the evaluation task group and were presented at the 2017 IAPWS meeting in Kyoto.

2. The work on a new mixed gas hydrate model consistent to reference equations of state continues. This work started as a collaboration of Ruhr-Universität Bochum (Prof. Dr. Roland Span, Dr. Andreas Jäger) and the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš). The work is now carried on as a collaboration of Ruhr-Universität Bochum (Prof. Dr. Roland Span, Sebastian Hielscher), the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš), and TU Dresden (Prof. Dr. Cornelia Breitkopf, Dr. Andreas Jäger). The model for CCS-relevant pure hydrate formers was recently successfully modified in order to allow the calculation of mixed gas hydrates, which resulted in a publication by Hielscher et al. (2018) and another planned publication for this year.

Recent Publications

o Herrig, S.; Thol, M.; Harvey, A.H.; Lemmon, E.W.:
A Reference Equation of State for Heavy Water,
J. Phys. Chem. Ref. Data (2018), submitted.

o Hielscher, S.; Vinš, V.; Jäger, A.; Hrubý, J.; Breitkopf, C.; Span, R.:
A New Approach to Model Mixed Hydrates,
Fluid Phase Equilib. 459 (2018), 170–185.

Ruhr University Bochum
Faculty of Mechanical Engineering, Chair of Thermodynamics
Prof. em. Dr. Dr. e. h. Wolfgang Wagner

Project

1. Preparation of the 3rd edition of the book "International Steam Tables".

Recent Publications

o 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 Energy Solutions, Erlangen
Michael Rziha

Projects

1. Development of new Technical Guidance Documents:
   o Air In-Leakage in Steam Water Cycles. Finally developed, so that the release can be expected in 2018
   o Ensuring the Integrity and Reliability of Demineralized Makeup Water Supply to the Unit Cycle. TGD is drafted, but still some work needs to be done. Release is expected by 2019
   o Film Forming Products. Following the release of the IAPWS TGD on FFP for Fossil and Combined Cycle Plants and the IAPWS International Conference on FFP in Lucerne and a 2nd conference in Prague in spring 2018, IAPWS will be developing two new TGD on FFP:
      a) Application of Film Forming Products in Nuclear Plants.
      b) Application of Film Forming Products in Industrial Plants.
   o Both TGD's are progressing, however still some work to be done, so release is not expected before 2019.

2. Developing of white papers as basis for future technical guidance documents
   o Monitoring Corrosion Products in Flexible (cycling and two-shifting) Plants. White paper is developed for presentation at the 2017 Meeting. TGD will be further developed based on this input.
   o Aspects of Geothermal Steam Chemistry. A White Paper for the 2017 Meeting is in preparation. This will be used to determine if a TGD can be developed.

Highlight:
   o IEC has finally agreed to withdraw their standard IEC 61370 Ed 1.0: 2002 Steam turbines - Steam purity in favor of IAPWS TGD5-13, due to the fact that the IAPWS TGD on steam purity is the most modern, state of the art and international accepted guidance on this topic. This is underlining once more the huge international leadership of IAPWS on aspects of high-temperature steam, water and aqueous mixtures relevant to thermal power cycles.
   o A so called category C liaison (which is some sort of loose liaison, just for exchange of information) between IEC - MT12 and IAPWS PCC Working Group will be established.

Siemens Energy Solutions, Erlangen
Ingo Weber, Stefan Bennoit, Julien Bonifay

Projects

1. Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code KRAWAL
   o The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the heat cycle code KRAWAL which is used worldwide by Siemens.
   o The computing time consumption of KRAWAL has been significantly reduced.

Recent Publications
   o 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. Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code EBSILON
   - o The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the heat cycle code EBSILON which is used worldwide by the power industry.
   - o The computing time consumption of EBSILON has been significantly reduced.

Recent Publications

   - o 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, Faculty of Mechanical Science and Engineering,
Thermodynamics
Prof. Dr. Cornelia Breitkopf
Dr. Andreas Jäger, Dr. Tommy Lorenz, Erik Mickoleit

Projects:

1. The work on a new mixed gas hydrate model consistent to reference equations of state continues. This work started as a collaboration of Ruhr-Universität Bochum (Prof. Dr. Roland Span, Dr. Andreas Jäger) and the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš). The work is now carried on as a collaboration of Ruhr-Universität Bochum (Prof. Dr. Roland Span, Sebastian Hielscher), the Institute of Thermomechanics of the CAS (Dr. Jan Hrubý, Dr. Václav Vinš), and TU Dresden (Prof. Dr. Cornelia Breitkopf, Dr. Andreas Jäger). The model for CCS-relevant pure hydrate formers was recently successfully modified in order to allow the calculation of mixed gas hydrates, which resulted in a publication by Hielscher et al. (2018) and another planned publication for this year.

2. Molecular simulations of volumetric properties and cage occupancies of gas hydrates in different crystal structures have been conducted and are ongoing work (Dr. Tommy Lorenz, Dr. Andreas Jäger). Properties of gas hydrate formers in structures that these hydrate formers do not form, if they are in a binary mixture with water, are important for the development of a model for mixed hydrates. As these quantities cannot be obtained experimentally, simulations are a viable option. First results will be presented on the 17th ICPWS in Prague (2018).

3. A new predictive mixing rule for the multi-fluid mixture model was developed and published (Jäger et al. (2018)). The new mixture model involves a theoretically based departure function, which allows for the combination of the multi-fluid mixture model with excess Gibbs energy models, like UNIFAC or COSMO-SAC. The application of this new model to mixtures containing water is ongoing work (Dr. Andreas Jäger, Erik Mickoleit). Results of the new model will be presented on the 17th ICPWS in Prague (2018).

Recent Publications

- o Hielscher, S.; Vinš, V.; Jäger, A.; Hrubý, J.; Breitkopf, C.; Span, R.:
  A New Approach to Model Mixed Hydrates.
  Fluid Phase Equilib. 459, 170–185 (2018).

- o Jäger, A.; Bell, I.H.; Breitkopf, C.:
  A theoretically based departure function for multi-fluid mixture models, Fluid Phase Equilib. 469, 56–69 (2018).

University of Rostock, Rostock
Institute of Chemistry, Department of Physical Chemistry
Dr. Robert Hellmann

Project

1. *Ab-initio* Calculations for Transport Properties of Water and Aqueous Mixtures.

Recent Publications
- o Hellmann, R.:
  Cross Second Virial Coefficient and Dilute Gas Transport Properties of the (H_2O+CO_2) System from First-Principals Calculations,
  Fluid Phase Equilib. (2018), submitted.

VGB PowerTech e.V., Essen
Dr. Andreas Wecker

Project

1. *Development of a new VGB- standard*: Chemical Feeding and Feed Systems for Water/Steam Circuits.
   o This VGB-Standard supplements the VGB Standards for "Feed Water, Boiler Water and Steam Quality for Power Plants / Industrial Plants" and VGB-Standard "Sampling and Physico-Chemical Monitoring of Water and Steam Cycles" and contains recommendations for the correct location, design and instrumentation as well as operation and maintenance of chemical feed equipment in the water/steam circuit. It was published in July 2018.

Zittau/Görlitz University of Applied Sciences
Department of Technical Thermodynamics
Prof. Dr. Hans-Joachim Kretzschmar, Dr. Sebastian Herrmann, Dr. Matthias Kunick

Projects

1. Development of fast property calculation algorithms based on spline interpolation
   o 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:
   o Non-stationary thermo-hydraulic code ATHLET of the German Society of Global Research for Safety GRS
   o Non-stationary thermo-hydraulic codes SubChanFlow and TwoPorFlow of the Karlsruhe Institute of Technology KIT
   o Non-stationary thermo-hydraulic code RELAP-7 of the Idaho National Laboratory INL
   o Heat-cycle simulation program EBSILON of STEAG Energy Services
   o Heat-cycle simulation program KRAWAL of Siemens Energy Solutions
   o Non-stationary heat-cycle simulation program DYNAPLANT of Siemens Energy Solutions.

3. Development of algorithms for the transport properties of moist air, ASHRAE Research Project 1767.

4. Preparation of a new ASHRAE standard for calculating moist air properties, ASHRAE Project SPC 213P.

5. Reworking on the 3rd edition of the book "International Steam Tables".

Recent Publications
   o 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.
   o Kunick, M.:
   Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL).
   Fortschritt-Berichte VDI, Reihe 6 Energietechnik, Nr. 618 (2018).

- o Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.
  N.N. (2018), in preparation.
- o Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air".
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