German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam

Report "Research in Progress 2015"

Baltic Sea Research Institute, Warnemuende
Dr. Rainer Feistel

Projects

1. Development of a draft "IAPWS Guideline on a Virial Equation for the Fugacity of H2O in Humid Air".

2. Leading preparation of the comprehensive paper for the Journal Metrologia:
   Metrological challenges for measurements of key climatological observables: Oceanic salinity and pH, and atmospheric humidity.

Publications:

- R Feistel, J W Lovell-Smith, P Saunders and S Seitz:
  Uncertainty of Empirical Correlation Equations.
  Submitted to Metrologia, 26 May 2015.

- R Feistel, R Wielgosz, S A Bell, M F Camões, J R Cooper, P Dexter, A G Dickson, P Fisicaro, A H Harvey, M Heinonen, O Hellmuth, H-J Kretzschmar, J W Lovell-Smith, T J McDougall, R Pawlowicz, P Ridout, S Seitz, P Spitzer, D Stoica and H Wolf:
  Metrological challenges for measurements of key climatological observables:
  Oceanic salinity and pH, and atmospheric humidity. Part 1: Overview.
  REVIEW PAPER. Submitted to Metrologia, 18 May 2015.

- R Pawlowicz, R Feistel, T J McDougall, P Ridout, S Seitz, H Wolf:
  Metrological challenges for measurements of key climatological observables, Part 2:
  Oceanic salinity. To be submitted to Metrologia.

- A G Dickson, M F Camões, P Spitzer, P Fisicaro, D Stoica, R Pawlowicz and R Feistel:
  Metrological challenges for measurements of key climatological observables, Part 3:
  Seawater pH. To be submitted to Metrologia.

- J W Lovell-Smith, R Feistel, A H Harvey, O Hellmuth, S A Bell, M Heinonen, J R Cooper:
  Metrological challenges for measurements of key climatological observables, Part 4:
  Atmospheric relative humidity. To be submitted to Metrologia.

- Feistel, R., Lovell-Smith, J.W., Hellmuth, O. (Proposers):
  Guideline on a Virial Equation for the Fugacity of H2O in Humid Air.
  The International Association for the Properties of Water and Steam.
  Stockholm, Sweden, July 2015, to be adopted.

- Feistel, R. (2015):
  Salinity and relative humidity: climatological relevance and metrological needs.
  Acta Imeko, in press.

- Feistel, R., Lovell-Smith, J.W., Hellmuth, O. (2015):
  Virial Equation for the Fugacity of Water in Humid Air.
  International Journal of Thermophysics 36, Issue 1, pp. 44-68.

- Rainer Feistel, Jeremy W. Lovell-Smith, Olaf Hellmuth (2015):
  Erratum to: Virial Approximation of the TEOS-10 Equation for the Fugacity of Water in Humid Air.
  International Journal of Thermophysics 36, Issue 1, p. 204

- Kretzschmar, H.-J., Herrmann, S., Feistel, R., Wagner, W.:
  The International IAPWS Formulation for the Thermodynamic Properties of Seawater for Desalination Processes.
  The International Desalination Association World Congress on Desalination and Water Reuse 2015, San Diego, CA, USA, Accepted (2015).
- Kretzschmar, H.-J., Feistel, R., Wagner, W., Miyagawa, K., Harvey, A.H., Cooper, J.R., Hiegemann, M., Blangetti, F.L., Orlov, K.A., Weber, I., Singh, A. Herrmann, S.:
  The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater.
  Desalination and Water Treatment xx, 1–23, doi: 10.1080/19443994.2014.925838, Published online (2014).
- Trevor J. McDougall, Paul M. Barker, Rainer Feistel, Ben K. Galton-Fenzi:
  Melting of ice and sea ice into seawater, and frazil ice formation.
  Journal of Physical Oceanography 44, 1751-1775, DOI: 10.1175/JPO-D-13-0253.1 (2014).

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

Project

Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the CFD Code TRACE

- The draft "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, cf. [1].
- On this basis the implementation has been further improved, especially regarding the software architecture, solution algorithm and boundary treatment.
- 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.

Paper

- Kunick, M., Kretzschmar, H.-J., di Mare, F., Gampe, U.:
  CFD Analysis of steam turbines with the IAPWS standard on the Spline-Based Table Look-Up Method (SBTL) for the fast calculation of real fluid properties.
  In *Turbine Technical Conference and Exposition: Proceedings of ASME Turbo Expo 2015*, 2015.

German Research Centre for Geosciences GFZ
Section 4.1 - Reservoir Technologies
Dr. Harald Milsch, Ulrike Hoffert

Projects

1. Measurements of density, viscosity and electrical conductivity of pure and mixed NaCl and $CaCl_2$ aqueous solutions at 0.1 MPa and 20-80°C
2. Evaluation of mixing rules for thermophysical properties of ternary $NaCl-CaCl_2$ aqueous solutions
3. Set-up and evaluation of a capillary-type high pressure-high temperature viscometer for aqueous electrolyte solutions at up to 50 MPa and 200°C

Publications

- Milsch, H., Hoffert, U., Hofmann, H. (2015): Data Gaps in Thermophysical Fluid Data for Geothermal Applications. Proceedings World Geothermal Congress, Melbourne, Australia, Paper 16028
- Hoffert, U. and Milsch, H. (2015): Experimental Investigations on the Thermophysical Properties of Synthetic Geothermal Fluids. Proceedings World Geothermal Congress, Melbourne, Australia, Paper 16030

Helmholtz Centre for Environmental Research –UFZ , Limnophysics Group, Magdeburg, Dr. Bertram Boehrer

Project

Density and electrical conductivity in limnic waters:

- A practical approach to lake water density from electrical conductivity and temperature
- Calculating conductance of acidic lake waters
- Accuracy of lake water density calculated from molar volumes: RHOMV

Book Publication

- Boehrer B.: Chapter 3.1 Physical properties of acidic pit lakes IN: Geller W., Schultze M., Kleinmann R., Wolkersdorfer C.:
  In: Acidic pit lakes.
  Springer, Heidelberg, 23-42 (2013)

Leibniz Institute for Tropospheric Research, Leipzig Dr. Olaf Hellmuth

Publications

- Hellmuth, O., R. Feistel, J. Lovell-Smith and J. Kalova, 2015:
  Metrological Aspects of Humidity: State of Discussion on Common Positions, Challenges, and Needs.
  Technical Report of the Joint BIPM, CCT-WG6/CCQM and JCS Workshop on Hygrometry, held during the 16th International Conference on the Properties of Water and Steam 2013 (ICPWS 2013), Greenwich, UK. Online available:
  http://www.teos-10.org/pubs/ICPWS2013_WS_TechnicalReport_Humidity_20150211primo.pdf
- Feistel, R., Lovell-Smith, J.-W., O. Hellmuth:
  Virial Approximation of the TEOS-10 Equation for the Fugacity of Water in Humid Air.
  Int J Thermophys (2015) 36:44–68, DOI 10.1007/s10765-014-1784-0
- Hellmuth, O., Shchekin, A. K.: Determination of interfacial parameters of a soluble particle in a nonideal solution from measured deliquescence and efflorescence humidities.
  Atmos. Chem. Phys., 15, 3851-3871, 2015
  www.atmos-chem-phys.net/15/3851/2015/, doi:10.5194/acp-15-3851-2015
- R Feistel, R Wielgosz, S A Bell, M F Camões, J R Cooper, P Dexter, A G Dickson, P Fisicaro, A H Harvey, M Heinonen, O Hellmuth, H-J Kretzschmar, J W Lovell-Smith, T J McDougall, R Pawlowicz, P Ridout, S Seitz, P Spitzer, D Stoica and H Wolf:
  Metrological challenges for measurements of key climatological observables: Oceanic salinity and pH, and atmospheric humidity. Part 1: Overview.
  Revised version, submitted for publication in Metrologia

- J W Lovell-Smith, R Feistel, A H Harvey, O Hellmuth, S A Bell, M Heinonen, J R Cooper:
  Metrological challenges for measurements of key climatological observables, Part 4:
  Atmospheric relative humidity
  Revised version, submitted for publication in Metrologia

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

Projects:

1. Improvement of accurate models available for CCS-relevant mixtures. Within this project humid mixtures are of particular interest, since existing models from the GERG-2008 package for natural gases are not designed for higher concentrations of water. A first version of this new-mixture model was recently submitted to the Journal of Chemical Thermodynamics and will be published soon. Software enabling the application of the latest version of our property models has been made available and is by now used by more than 50 groups worldwide (both in academia and in industry).

2. The work on models describing hydrate formation has been continued in cooperation with Dr. V. Vins and Dr. J. Hruby. The Ph.D. thesis of A. Jäger has been completed. Three journal articles describing the latest status of the hydrate model in detail will be submitted within the next few weeks. S. Hielscher will continue this work at RUB; funding for this important project has been granted by the German Science Foundation (DFG).

3. 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. Harvey and Dr. E. W. Lemmon at NIST in Boulder. The work on the new equation of state is still proceeding. It is enhanced by new highly accurate measurements of the speed of sound in the liquid phase. The experiments were performed by means of the single-burst pulse-echo technique in the speed of sound laboratory at RUB. The current status of the new equation of state as well as the speed of sound measurements has been presented at the 19th Symposium on Thermophysical Properties in Boulder, Colorado. The new equation of state will be validated over the next months.

Publications

- Gernert, J.; Span, R.:
  EOS-CG: A Helmholtz energy mixture model for humid gases and CCS mixtures.
  J. Chem. Therm., In press (2015)

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

Projects

1. Working for the article "Behavior of IAPWS-95 from 250 K to 300 K and Pressures up to 400 MPa: Evaluation Based on Recently Derived Property Data."

2. Working for the report "Behavior of IAPWS-95 from 250 K to 300 K and Pressures up to 400 MPa: Evaluation Based on Recently Derived Property Data." The results will be presented at the IAPWS Annual Meeting in Stockholm 2015.

Publications

- Wagner, W., Thol, M.:
  Behavior of IAPWS-95 from 250 K to 300 K and Pressures up to 400 MPa: Evaluation Based on Recently Derived Property Data.
  Submitted to J. Phys. Chem. Ref. Data (2015).

- Kretzschmar, H.-J. Feistel, R., Wagner, W., Miyagawa, K., Harvey, A. H., Cooper, J. R., Hiegemann, M. Blangetti, F. L., Orlov, K. A., Weber, I., Singh, A., Herrmann, S.:
  The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater.
  Desalination and Water Treatment (2014), 1-23.

- Kretzschmar, H.-J., Herrmann, S., Feistel, R., Wagner, W.:
  The International IAPWS Formulation for the Thermodynamic Properties of Seawater for Desalination Processes.
  The International Desalination Association World Congress on Desalination and Water Reuse 2015, San Diego, CA, USA. Accepted (2015)

Siemens Energy Solutions, Erlangen
Michael Rziha

Projects

1. Amendments and Revisions of the following three Technical Guidance Documents:
   - Technical Guidance Document – 2015 Revision:
     Instrumentation for monitoring and control of cycle chemistry for the steam-water circuits of fossil-fired and combined cycle power plants
   - Technical Guidance Document – 2015 Revision:
     Phosphate and NaOH treatments for the steam-water circuits of drum boilers of fossil and combined cycle/HRSG power plants
   - Technical Guidance Document – 2015 Revision:
     Volatile treatments for the steam-water circuits of fossil and combined cycle/HRSG power plants.

   All three documents are ready to be adopted by the EC in Stockholm.

2. Developing of a draft for a new technical guidance document "HRSG HP Evaporator Sampling for Internal Deposit Determination", which will be discussed within PCC Working Group during the Stockholm meeting.

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
   - The draft "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.
   - The computing time consumption of KRAWAL has been significantly reduced.

2. Implementation of the fast steam property spline-interpolation algorithms into the non-stationary power-plant simulation code DYNAPLANT
   - The draft "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 non-stationary power-plant simulation code DYNAPLANT.
   - The computing time consumption of DYNAPLANT has been significantly reduced.

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

Project

Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code EBSILON
   - The draft "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.
   - The computing time consumption of EBSILON has been significantly reduced.

Zittau/Goerlitz University of Applied Sciences
Department of Technical Thermodynamics
Prof. Dr. Hans-Joachim Kretzschmar

Projects

1. Development of fast property algorithms based on spline interpolation
   - Spline property algorithms were developed for functions of the variables specific volume and specific internal energy (v,u) and related inverse functions for water and steam based on the scientific formulation IAPWS-IF95.
   - The range of validity of the spline-property functions based on IAPWS-IF97 has been expanded to metastable subcooled steam and metastable superheated liquid water.
   - Spline property algorithms have been developed for functions of the variables specific volume an specific enthalpy (v,h) as well as for the related inverse functions for water and steam based on the industrial formulation IAPWS-IF97.
   - The draft "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 expanded to IAPWS-95 and the metastable subcooled steam region of IAPWS-IF97
   - The evaluation by the IAPWS Evaluation Task Group has been supported.

2. Application of the developed spline algorithms for calculating thermodynamic properties

   The developed spline property algorithms have been implemented into the following process simulation codes:
   - Non-stationary thermo-hydraulic cycle program RELAP-7 of the Idaho National Institute INL
   - Heat cycle simulation program EBSILON of STEAG Energy Services
   - Heat cycle simulation program KRAWAL of Siemens Energy Solutions
   - Non-stationary heat cycle program DYNAPLANT of Siemens Energy Solutions.

Recent Publications

- Kunick, M.; Kretzschmar, H.-J.; di Mare, F.; Gampe, U.:
  CFD Analysis of steam turbines with the IAPWS standard on the Spline-Based Table Look-Up Method (SBTL) for the fast calculation of real fluid properties.
  In: Turbine Technical Conference and Exposition: Proceedings of ASME Turbo Expo (2015).

- Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.:
  Simulation instationärer Prozesse und CFD in Dampfturbinen mithilfe eines neuen Spline-basierten Stoffwert-Berechnungsverfahrens (Simulation of non-stationary processes and CFD in steam turbines using the new spline-based property calculation method).
  In: Kraftwerkstechnik 2014, Eds. Beckmann, M. und Hurtado, A., Verlag Saxonia, Freiberg, S. 515-526 (2014)

- Kretzschmar, H.-J.; Feistel, R.; Wagner, W.; Miyagawa, K.; Harvey, A. H.; Cooper, J. R.; Hiegemann, M.; Blangetti, F. L.; Orlov, K. A.; Weber, I.; Singh, A.; Herrmann, S.:
  The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater.
  Desalination and Water Treatment, 2014, 1-23.

- Kretzschmar, H.-J.; Herrmann, S.; Feistel, R.; Wagner, W.:

  The International IAPWS Formulation for the Thermodynamic Properties of Seawater for Desalination Processes.

  In Proceedings of the International Desalination Association World Congress on Desalination and Water Reuse, San Diego CA, Accepted (2015).

- Kraft, I.; Kretzschmar, H.-J.:
  Reale Fluide und Grundlagen der Wärmeübertragung, Lernheft THD101: Grundlagen der Technischen Thermodynamik (Real fluids and the basics of heat transfer, Learning booklet THD101: Basics of Technical Thermodynamics).
  AKAD, Bildungsgesellschaft mbH, Art.-Nr. 10880 (2014).

- Kraft, I.; Kretzschmar, H.-J.:
  Gasgemische und feuchte Luft, Lernheft THD102: Grundlagen der Technischen Thermodynamik (Gas mixtures and humid air, Learning booklet THD102: Basics of Technical Thermodynamics).
  AKAD, Bildungsgesellschaft mbH (2014). Art.-Nr. 11112 (2014).

- Kraft, I.; Kretzschmar, H.-J.:
  Verbrennungsrechnung, Lernheft THD103: Grundlagen der Technischen Thermodynamik (Combustion calculation, Learning booklet THD103: Basics of Technical Thermodynamics).
  AKAD, Bildungsgesellschaft mbH, Art.-Nr. 11113, (2014).

- Kretzschmar, H.-J.; Stoecker, I.; Kunick, M.; Herrmann, S.; Nicke, M.:
  Calculation of Thermodynamic Properties on Pocket Calculators, Smart Phones, Tablets, Notebooks, and Online.
  In: Proceedings of the Congress INFORINO, Trudi Mechdunarodny Nauchno-Metodichesky Konferenzy, Isdatjelstvo, Moskva 2014, PP. 179-182 (2014), ISBN.: 978-5-7046-1535-4.

- Feistel, R.; Wielgosz, R.; Bell, S. A.; Camões, M. F.; Cooper, J. R.; Dexter, P.; Dickson, A. G.; Fisicaro, P.; Harvey, A. H., Heinonen, M.; Hellmuth, O.; Kretzschmar, H.-J.; Lovell-Smith, J. W.; McDougall, T. J.; Pawlowicz, R.; Ridout, P.; Seitz, S.; Spitzer, P.; Stoica, D.; Wolf, H.:
  Metrological challenges for measurements of key climatological observables: Oceanic salinity and pH, and atmospheric humidity. Part 1: Overview.

Revised version, submitted for publication in Metrologia.