German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam

Report "Research in Progress 2014"

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.

Book Publications

Feistel, R. Tailleux, R., McDougall, T. (Eds.): Thermophysical Properties of Seawater. Ocean Science Special Issue. Copernicus Publications, Göttingen (2013), ISSN 1812-0784

Hellmuth, O., Khvorostyanov, V.I., Curry, J.A., Shchekin, A.K., Schmelzer, J.W.P., Feistel, R., Djikaev, Y.S., Baidakov, V.G.: Selected Aspects of Atmospheric Ice and Salt Crystallisation. Review Series on Selected Topics of Atmospheric Sol Formation, Volume 1. Nucleation Theory and Applications, Joint Institute for Nuclear Research, Dubna, Russia (2013), ISBN 978-5-9530-0349-0

Papers

Feistel, R., Lovell-Smith. J. (proposers): Guideline on a Virial Equation for the Fugacity of H2O in Humid Air. The International Association for the Properties of Water and Steam, Greenwich, UK, September 2013, submitted

Safarov, J., Berndt, S., Millero, F., Feistel, R., Heintz, A., Hassel, E. (2013): (p,rho,T) Properties of seawater at brackish salinities: Extensions to high temperatures and pressures. Deep-Sea Research I, 78 (2013) 95–101

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.

Leibniz Institute for Tropospheric Research, Leipzig
Dr. Olaf Hellmuth

Project

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

Book Publication

Hellmuth, O., Khvorostyanov, V.I., Curry, J.A., Shchekin, A.K., Schmelzer, J.W.P., Feistel, R., Djikaev, Y.S., Baidakov, V.G.: Selected Aspects of Atmospheric Ice and Salt Crystallisation. Review Series on Selected Topics of Atmospheric Sol Formation, Volume 1. Nucleation Theory and Applications, Joint Institute for Nuclear Research, Dubna, Russia (2013), ISBN 978-5-9530-0349-0

Papers:

Shchekin, A.K., Shabaev, I.V., Hellmuth, O.,
Thermodynamic and kinetic theory of nucleation, deliquescence and efflorescence transitions in the ensemble of droplets on soluble particle,
J. Chem. Phys. 138, 054704 (2013); doi: 10.1063/1.4789309

PTB Braunschweig
Dr. Petra Spitzer

Project

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

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

The group chaired by Prof. Span has been actively involved in a number of research projects related to CO_2-rich mixtures as are typical for power generation with carbon capture and storage (CCS), to hydrate formation and to heavy water. The work of Prof. Span primarily addresses the

- improvement of the experimental data base available for CCS-relevant mixtures. Experimental programs are financed by BIGCCS (Norwegian Science Foundation) and IMPACTS (EU). Measurements include density, speed of sound and dew point of CO_2 rich mixtures and other relevant binary systems. In September 2013 the corresponding experimental equipment was moved into new, modern laboratories in a new building. Though this new environment is a remarkable improvement, complications related mostly to the air conditioning of the new laboratories have not been completely yet. Much work has had to be invested into the new laboratories.
- improvement of accurate models available for CCS-relevant mixtures. The main foci of this work have been the development of improved mixing models and a consistent description of complex phase equilibria [1], including the formation of hydrates and other solid phases. This work is linked to close

co-operations with the group of Dr. J. Hruby at the Czech Academy of Sciences and with Dr. E. W. Lemmon at NIST in Boulder.

- a chapter in a book on CCS [2] has been written to raise the awareness of thermodynamic property-related issues in CCS.
- 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. Work on the new equation of state is proceeding slowly. New experimental data are expected for the vapor pressure of heavy water (from NIST) and for speed of sound in liquid heavy water (from Bochum's speed of sound laboratory). Once these data are available the equation of state can be finalized.

Many aspects of the work on CCS-relevant mixtures are closely related to work on properties of natural gases, particularly in conjunction with LNG processing. However, this work is not considered within the primary scope of IAPWS.

[1] *J. Gernert, A. Jäger, R. Span:* Calculation of Phase Equilibria for Multi-Component Mixtures Using Highly Accurate Helmholtz Energy Equations of State. Fluid Phase Equilibria, 2014.

[2] *K. Görner (Ed.):* CO_2: Abtrennung, Speicherung, Nutzung. Springer (2014).

Related Papers

[3] *R. Span, J. Gernert, A. Jäger:* Accurate Thermodynamic-Property Models for CO_2-Rich Mixtures. Energy Procedia, 2013.

[4] *H.G. Jacob Stang, J.P. Jakobsen, Ø. Wilhelmsen, R. Span:* CO_2 Mix Project: Experimental Determination of Thermo Physical Properties of CO_2-Rich Mixtures. Energy Procedia, 2013.

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

Projects

1. Working for the report "Possible Improvements of the Uncertainty Estimates of IAPWS-95" within the Task Group "Uncertainty Estimates of IAPWS-95" for the Working Group "Thermophysical Properties of Water and Steam." The results will be presented at the IAPWS Annual Meeting in Moscow 2014.
2. Preparatory work for the article "Behavior of the IAPWS-95 Formulation for Temperatures from 253 K to 303 K at Pressures up to 400 MPa."

Publications

- Wagner, W., Dauber, F., Kretzschmar, H.-J., Mareš, R., Miyagawa, K., Span, R. Extended equation for region 5 of the Industrial Formulation IAPWS-IF97. Proceedings of the International Conference on the Properties of Water and Steam, September 2013, University of Greenwich, London, UK, Institution of Mechanical Engineers, London SW1H 9JJ, UK.
- 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. Accepted for publication in Desalination and Water Treament (2014).

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

Project

Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the Heat Cycle 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.

STEAG Energy Services, Zwingenberg
Reiner Pawellek

Project

Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the Heat Cycle 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.

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

Projects

1. Development of Fast Property Algorithms Based on Spline Interpolation
   - The algorithms for the fast spline-interpolation method have been developed and applied to the calculation of thermodynamic properties of steam and water in CFD and non-stationary calculations.
   - 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 completed and evaluated.
2. Industrial Calculation of the Thermodynamic Properties for Seawater
   - The paper "The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater" has been completed and submitted to the Journal Desalination and Water Treatment.

Recent Publications

- Wagner, W., Dauber, F., Kretzschmar, H.-J., Mareš, R., Miyagawa, K., Span, R. Extended equation for region 5 of the Industrial Formulation IAPWS-IF97. Proceedings of the International Conference on the Properties of Water and Steam, September 2013, University of Greenwich, London, UK, Institution of Mechanical Engineers, London SW1H 9JJ, UK.
- 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. Accepted for publication in Desalination and Water Treatment (2014).