# **German National Committee to IAPWS**

# **Research Activities on the Thermodynamic Properties of Water and Steam**

# **Report "Research in Progress 2013"**

## Baltic Sea Research Institute, Warnemuende

### Dr. Rainer Feistel

#### **Book Publication**

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)

### 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

Kretzschmar, H.-J., Feistel, R., Wagner, W., Miyagawa, K., Harvey, A.H., Cooper, J.R., Hiegemann, M., Herrmann, S. (proposers): Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater. 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

# Leibniz Institute for Tropospheric Research, Leipzig Dr. Olaf Hellmuth

**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)

# 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 fast spline-interpolation methods was developed and applied to the calculation of thermodynamic properties of steam and water in CFD and non-stationary calculations.
  - A Draft "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (STM)" has been prepared.
- 2. Industrial Calculation of the Thermodynamic Properties for Seawater
  - The Draft "IAPWS Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater" has been evaluated.

The belonging paper for the Journal Desalination: "The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater" has been prepared.

- 3. Steam Tables for Water and Steam, VDI Wärme Atlas 2012
  - Section D2.1 "Stoffwerte für Wasser und Wasserdampf" (Properties of Water and Steam) of the VDI-Wärme Atlas 2012 (VDI-Heat Atlas), 11th German Edition has been completed. The corresponding steam tables are calculated based on the Industrial Formulation IAPWS-IF97 and the current IAPWS formulations for the transport properties and other properties.
- 4. Property Libraries for Calculating Heat Cycles
  - The property library LibIF97\_META for metastable steam has been prepared.
  - A steam tables App for Android smart phones and tablets has been developed.

#### **Recent Publications**

Wagner, W., Kretzschmar, H.-J.:

D2.1 Stoffwerte von Wasser und Wasserdampf, In: VDI-Wärmeatlas, 11. Auflage. Springer-Verlag, Berlin, 2013.

Herrmann, S.; Kretzschmar, H.-J.; Gatley, D.P.: In: 2013 ASHRAE HANDBOOK FUNDAMENTALS, SI and I-P Editions, Chapter 1

## PSYCHROMETRICS,

Table 2 Thermodynamic Properties of Moist Air at Standard Atmospheric Pressure. Table 3 Thermodynamic Properties of Water at Saturation.

American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta GA (2013), ISBN 978-1-936504-46-6, www.ashrae.org

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

The group chaired by Prof. Span has actively been involved in a number of research projects related to  $CO_2$ -rich mixtures as they 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 densities, speeds of sound and dew points of CO<sub>2</sub> rich mixtures and other relevant binary systems. An international workshop aiming at improved coordination of measurement programs was organized in January 2013.
- improvement of accurate models available for CCS-relevant mixtures. Main foci of this work have been the development of improved mixing models (1) and a consistent description of complex phase equilibria, including the formation of hydrates and other solid phases (2). 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.
- development of a new reference equation of state for heavy water (3). 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.

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 new Helmholtz energy model for humid gases and CCS mixtures. Dissertation, Ruhr-Universität Bochum (2013).

- (2) A. Jäger, Václav Vinš, J. Gernert, R. Span und J. Hrubý: Phase equilibria with hydrate formation in H<sub>2</sub>O + CO<sub>2</sub> mixtures modeled with reference equations of state. Fluid Phase Equilibria 338, 100-113 (2013).
- (3) S. Herrig:

Development of a new equation of state for heavy water. Master Thesis, Ruhr-Universität Bochum (2013).

**Related Papers** 

F. Dauber und R. Span:

Modeling liquefied-natural-gas processes using highly accurate property models. Applied Energy 97, 822-827 (2012).

R. Span, J. Gernert und A. Jäger:

Accurate thermodynamic-property models for CO<sub>2</sub>-rich mixtures.

Proceedings 11<sup>th</sup> Greenhouse Gas Technology Conference, Kyoto (2012). Energy Procedia 37, 2914-2922 (2013).

S. W. Løvseth, G. Skaugen, J. Stang, J. P. Jakobsen, Ø. Wilhelmsen, R. Span und R. Wegge: CO2Mix Project: Experimental determination of thermophysical properties of CO2-rich mixtures.

Proceedings 11<sup>th</sup> Greenhouse Gas Technology Conference, Kyoto (2012).

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

Projects

- Steam Tables for Water and Steam, VDI Wärme Atlas 2012 Section D2.1 "Stoffwerte für Wasser und Wasserdampf" (Properties of Water and Steam) of the VDI-Wärme Atlas 2012 (VDI-Heat Atlas), 11th German Edition, has been completed. The corresponding steam tables are calculated based on the Industrial Formulation IAPWS-IF97 and the current IAPWS formulations for the transport properties and other properties.
- 2. The behavior of the IAPWS-95 Formulation in the liquid region of water near the melting line at high pressures was investigated. A corresponding report on this matter will be presented on the IAPWS Meeting in Boulder 2012 in the Session of the IAPWS Working Group "Thermophysical Properties of Water and Steam" (TPWS).

**Recent Publications** 

- Wagner, W., Riethmann, T., Feistel, R., Harvey, A. H.: New equations for the melting pressure and sublimation pressure of H<sub>2</sub>O ice Ih. J. Phys. Chem. Ref. Data 40 (2011), 043103-1 - 043103-11 (online publication 05.12.2011).
- 1. Project: Investigations of the behavior of the IAPWS-95 formulation at temperatures from 250 K to 300 K and pressures up to 400 MPa

The background for this work was the article Holten V., C. E. Bertrand, M. A. Anisimov, and J. V. Sengers: Thermodynamics of supercooled water. J. Chem. Phys. 136 (2012), 094507-1 – 094507-18, where the behavior of IAPWS-95 at low temperatures and high pressures was criticized. The results of these investigations are summarized in the report "Behavior of the IAPWS-95 formulation at temperatures of 250 K and to 300 K and pressures up to 400 MPa" by Wolfgang Wagner and Monika Thol, Report prepared for the Task Group "Subcooled Water" and the Working Group "Thermophysical Properties of Water and Steam" of the International Association for the Properties of Water and Steam, May 2013.

A corresponding paper will be given at the 16th International Conference on the Properties of Water and Steam, London, 2013; see the papers for this conference below.

2. Publications in the field "Properties of Water and Steam"

Wagner, W., Kretzschmar, H.-J.: D2.1 Stoffwerte von Wasser, In: VDI-Wärmeatlas, 11. Auflage, Springer-Verlag, Berlin, 2013.

*Wagner, W., Dauber, F., Kretzschmar, H.-J., Mareš, R., Miyagawa, K., Span, R.* Extended equation for region 5 of the Industrial Formulation IAPWS-IF97. Submitted to Proceedings of the International Conference on the Properties of Water and Steam, London, 2013.

## 3. Further publication

*Kunz, O., Wagner, W.* The GERG-2008 Wide-Range Equation of State for Natural Gases and Other Mixtures: An Expansion of GERG-2004. J. Chem. Eng. Data 57 (2012), 3032-3091 (online publication 31.10.2012).