

## **BRITISH AND IRISH ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM**

**A Member of the International Association for  
the Properties of Water and Steam**

# **BIAPWS**

**[www.biapws.org](http://www.biapws.org)**

Chair:	Mr. P. McCann, E.ON New Build & Technology Limited, Ratcliffe on Soar, NG11 0EE, UK
Vice-Chair	Mr. G. Aspinall, AMEC, 601 Faraday Street, Birchwood, Warrington, WA3 6GN, UK
Secretary	Dr M Robson, RWE npower Laboratory Building, TSG Ferrybridge, Knottingley, WF11 8PR, UK
Treasurer	Mr E G Huff, Plush Hill, All Stretton, Shropshire, SY6 6JP, UK

BIAPWS Annual Report 2012

### **1. Introduction**

The British and Irish Association for the Properties of Water and Steam (BIAPWS) is the UK and Ireland national committee of the International Association for the Properties of Water and Steam (IAPWS) and the representative body for Power Plant Chemistry in the UK and Ireland. BIAPWS is a not for profit organisation. This is the annual report of the activities of BIAPWS for the year to April 2012.

2011/12 has been another successful year for BIAPWS. Membership has remained strong, BIAPWS events have been well supported and the BIAPWS symposium and BIAPWS Award have both been successful. Preparations are progressing well for the 16<sup>th</sup> International Conference on the Properties of Water and Steam (ICPWS), which will be co-hosted by BIAPWS and the Institution of Mechanical Engineers (IMechE) at the University of Greenwich, 1-5 September 2013.

BIAPWS was pleased at the start of 2012 to welcome new holders of the roles of Chair, Vice-Chair and Secretary. BIAPWS would like to thank all the Officers who stepped down from their positions in 2012, however I would like to highlight our appreciation for the invaluable contributions to BIAPWS that Richard Harries has made over the years, as vice chair, chair and more recently secretary. We were also pleased to introduce an updated BIAPWS web-site in 2011 and our thanks go to our 'webmaster', Ken McGrath, for his diligent work towards this. BIAPWS finances remain in good stable condition and it is pleasing that, as a result, membership fees for sponsoring organisations have remained unchanged for the third year running. I would like to thank Eric Huff for his continuing excellent work as our Treasurer in helping to achieve this good state of financial health.

IAPWS request that National Committees provide, with their annual report, a listing of relevant technical publications that have originated from the respective nation/s during the year. The purpose of this request is to allow National Committees to share such lists and thereby widely

disseminate the international body of work being done on topics of interest to IAPWS and to IAPWS members. The list of publications for the UK and Ireland for the 2011/12 period is therefore provided in the Appendix to this report.

If you would like to know more about BIAPWS, feel free to contact one of the BIAPWS Officers listed above, visit our web site [www.biapws.org](http://www.biapws.org) or e-mail [contact.us@biapws.co.uk](mailto:contact.us@biapws.co.uk).

## **2. BIAPWS Membership**

BIAPWS membership has remained strong and BIAPWS is currently supported by nineteen industrial sponsors, six ordinary members and seven corresponding members. In 2011/12 BIAPWS was pleased to welcome AES and Watercare International as new industrial sponsors. BIAPWS committee meetings are held three times a year, and attendance at these continues to be very good, typically around twenty. BIAPWS committee meetings are preceded by a couple of technical presentations, which always generate a high level of interest. Industrial member's representatives are able to bring a colleague to the meeting to benefit from and contribute to the discussions.

BIAPWS has a strong membership representation in the area of power plant chemistry. However, other areas that are of relevance to IAPWS, for example the thermophysical properties of water and steam and the physical chemistry of aqueous solutions, are less well represented and BIAPWS remains keen to expand its individual membership in these areas.

I am very pleased to report that in 2012, BIAPWS formally agreed to new Statutes, the changes in which included the creation of a new individual membership category, that of Honorary Member. This category of membership is reserved for those BIAPWS members who have made a significant contribution to the achievements and aims of BIAPWS over an extended period. I am delighted to report that on completion of the changes to the Statutes, the following individuals were duly elected to the position of Honorary Member: Freddie Bakhtar, Malcolm Ball, Geoff Bignold, Jeff Cooper, Richard Harries, Eric Huff and Ken McGrath.

It was with great sadness that BIAPWS was informed of the sudden death, after a short illness, of Geoff Bignold in August 2012. Geoff was a former vice chair and chair of BIAPWS, an IAPWS Honorary Fellow, and was highly regarded internationally for his work and knowledge of power plant chemistry.

## **3. IAPWS Activities**

BIAPWS has continued to support IAPWS through its formal membership and participation in IAPWS activities. A number of BIAPWS committee members are represented on IAPWS working groups, in particular Power Cycle Chemistry (PCC). BIAPWS members of the PCC working group are also supporting the production of a new suite of IAPWS Technical Guidance Documents that are expected to provide a valuable resource to those involved in power cycle chemistry.

IAPWS holds annual meetings and BIAPWS members support these events by participating in the relevant IAPWS working groups. In addition, BIAPWS is represented on the executive committee of IAPWS. Every four or five years IAPWS holds the International Conference on the Properties of Water and Steam (ICPWS) in place of the annual meeting. The next such conference will be the 16<sup>th</sup> and this will be hosted by BIAPWS and held at the University of Greenwich, 1-5 September 2013. It has been over fifty years since this conference has been held in the UK and BIAPWS is looking forward to a welcome return to London, where the very first such conference was held in 1929. A BIAPWS sub-group is leading the work on ICPWS 16 in coordination with the IMechE, which is co-hosting the event with BIAPWS and has taken on the role of Conference Organiser. We are very grateful to the ICPWS sub-group, comprising Eric Huff, Hugh Lloyd and Jeff Cooper, and to the IMechE, for their work to make this important event a success. For more information on the Conference go to [www.icpws16.org/](http://www.icpws16.org/).

For further information on the activities of IAPWS, visit the IAPWS web site, [www.iapws.org](http://www.iapws.org).

#### **4. BIAPWS Award**

The BIAPWS Award is given annually by BIAPWS to qualifying students as a means of promoting awareness of the topics of interest to BIAPWS and their industrial application. In 2011 the BIAPWS award was co-sponsored by EDF Energy Nuclear Generation and the award recipient was David Docherty from Imperial College, London. The Award is given in the form of contributory funding by BIAPWS for a work experience placement for the student. David spent ten weeks with EDF Energy Nuclear Generation in Gloucester working on techniques to access look-up tables for steam / water properties when running computer simulations of transients in advanced gas-cooled reactors (AGRs). David gave excellent presentations on his work, firstly at the BIAPWS committee meeting in January 2012 and then at the BIAPWS Symposium in March 2012.

Many past BIAPWS Award winners have since gone on to full time employment in power generation, demonstrating significant success for the Award in attracting high calibre individuals to the industry.

BIAPWS has also continued to sponsor and judge prizes for energy related projects at a schools science fair in Hinckley, Leicestershire. We are currently looking for new opportunities to support ventures of this nature.

#### **5. BIAPWS Symposium**

The 14th BIAPWS Symposium, 'Progress in Environmental and Cycle Chemistry', took place at the Village Hotel, Nottingham, on 28-29 March 2012.

The Symposium consisted of two sessions: the first session on 28 March, 'Power Plant Fundamentals', was targeted at developing chemists and engineers with an interest in chemical operations and described the principles of cycle chemistry and boiler chemical cleaning. The second session on 29 March consisted of more detailed technical presentations on 'Environmental and Water Treatment Issues' and 'Power Plant Chemistry and Corrosion'.

This annual event continues to be very popular, with over eighty delegates attending the first session and over one hundred delegates attending the second session. This demonstrated not only the continued interest in the UK in developments in cycle chemistry and water treatment, but also the interest in more fundamental aspects. A summary report of the event was published in the journal *Power Plant Chemistry*, see *PPChem* 2012, 14(5), 298-305.

BIAPWS would like to extend its gratitude to all those who helped to make this event such a success.

## **6. BSI Representation**

In recent years BIAPWS has participated in formal Standards Committees of relevance to its members. As a result BIAPWS is currently represented on three British Standards Committees:

- PVE/2: Water Tube and Shell Boilers. This committee is of relevance to BIAPWS because it is the UK standards committee with responsibility for BS EN 12952-12:2003: Water-tube boilers and auxiliary installations - requirements for boiler feedwater and boiler water quality, and BS EN 12953-10:2003 Shell boilers - Requirements for feedwater and boiler water quality. BIAPWS has led on behalf of other European power plant chemistry specialists to lobby for these standards to be revised and improved. Whilst the European body responsible for these standards has agreed to their revision, there has not been any significant developments in 2011/12.
- CII/62: Treatment of water for boilers. This committee is of relevance to BIAPWS because it is the UK standards committee with responsibility for BS 2486:1997 Recommendations for treatment of water for steam boilers and water heaters. Currently, this committee is not active
- EH/3/6: Water quality - sampling. This committee is of relevance to BIAPWS because it is the UK standards committee with responsibility for BS 6068-6.7:1994 (ISO 5667-7:1993), Guidance on sampling of water and steam in boiler plants. BIAPWS is expecting to take a lead in revising this document in the forthcoming years and is currently looking at the best way to support the committee.

## **7. Interaction with Professional Organisations**

Because of the diverse nature of the interests of IAPWS, the areas of interest to BIAPWS overlap with the areas of interest of a number of professional bodies. As a result, BIAPWS has corresponded over the last year with a number of bodies with the aim of sharing information and closer working. BIAPWS is now represented on the Water Science Forum of the Royal Society of Chemistry and in 2012 Richard Hill joined BIAPWS as a corresponding member, representing the Water Subject Group of the Institution of Chemical Engineers (IChemE), for which Richard is a Committee member. BIAPWS is also interacting with the Power Industries Division of the IMechE with reference to the organisation of ICPWS 16.

## **8. Closing Remark**

In my last BIAPWS report, I would like to express my sincerest gratitude to all those individuals and organisations who contribute, sometimes in personal time, to the workings of BIAPWS and in support of BIAPWS activities. Without these contributions, BIAPWS would not be able to function effectively.

Dr. Andy Rudge

Chair (to January 2012), British & Irish Association for the Properties of Water and Steam  
July 2012

**APPENDIX: List of UK and Ireland Originated Reference Papers in areas of interest to IAPWS, published between April 2011 and March 2012:**

Adelina Henderson and David Brazil, “Failure Analysis of HP Feedwater Line Elbow”, PowerPlant Chemistry 2012, 14(2), 76-82

Richard J. Jones, “Generator Cooling Water Systems: Modelling Flammable Mixture Formation in Hydrogen Detraining Tanks”, PowerPlant Chemistry 2011, 13 (10), 614-620

Paul McCann and Mark Robson, “Proceedings of the BIAPWS 2011 Workshop and Symposium on Power Plant Chemistry”, PowerPlant Chemistry 2011, 13 (5)

Graham P. Quirk, Ian S. Woolsey, and Andy Rudge, “Use of Oxygen Dosing to Prevent Flow-Accelerated Corrosion in Advanced Gas-Cooled Reactors”, PowerPlant Chemistry 2011, 13 (4)

Bakhtar, F. and Zamri, M. Y., “On the Performance of a Cascade of Improved Nozzle Blades in Nucleating Steam - Part 3: Theoretical Analysis”, Proc. IMechE, Part C, Journal of Mechanical Engineering Science, 2011, 225 (C7), 1649-1671

C. –W. Lin and J. P. M. Trusler “The speed of sound and derived thermodynamic properties of pure water at temperatures between (253 and 473) K and at pressures up to 400 MPa”, J. Chem. Phys. 136, 094511 (2012)

## IAPWS Canadian National Committee

### Annual Report 2012

**Executive:** *David Guzonas (Chair); William Cook (Vice-Chair); Derek Lister (Secretary-Treasurer); Peter Tremaine (Member at Large); Melonie Myszczyzyn (Member at Large); CANDU Owners Group Representative (Steve McGee)*

**1. Canadian National Committee:** Dues for the Canadian National Committee (CNC) of IAPWS are supported by the National Research Council of Canada. This arrangement requires support and participation by a national organization representing industry. In 2004 the CANDU Owners Group took on this role on a trial basis, and in 2007 the CANDU Owners Group accepted this role for a five year term, including travel support for the academic members of the CNC. The CANDU Owners Group has been very supportive and proactive in supporting the CNC, and discussions are underway to renew their support for another five year term.

#### **2. NSERC/NRCan/AECL Generation IV Energy Technologies Program**

A major university-based program to study water chemistry in support of the development of the Canadian Supercritical Water-cooled Reactor concept (NSERC/NRCan/AECL Generation IV Energy Technologies Program) concluded Phase I in 2012. Phase II of this program, which will last for four years, started in 2012 and includes seven water chemistry projects that cover two main themes: a) corrosion product transport and deposition, and b) water radiolysis. The goal is to develop chemistry control strategies for the SCWR as well as recommend realistic chemistry conditions for corrosion testing in support of materials selection. The program also funds eight projects examining materials degradation phenomena (e.g., corrosion, stress corrosion cracking, creep) at temperatures up to 850 °C. A kick-off workshop was held in Saskatoon in 2012 June.

Research on high-temperature water chemistry being funded by this program includes:

**P. Tremaine (U. of Guelph):** Aqueous chemistry of metals and fission product under SCWR conditions.

**C. Pye (St. Mary's University):** Ab initio calculations on ionic hydration and complexation.

**W. Cook (U. of New Brunswick):** Corrosion product transport and deposition under SCWR conditions.

**I. Svishchev (Trent University):** Water chemistry, pH control and particle formation process in an SCWR.

**A. Anderson (St. Francis Xavier University):** Time-resolved investigations of metal oxide-water systems under conditions of extreme temperature, pressure and radiation.

**P. Percival (Simon Fraser University), K. Ghandi (Mount Allison University):** Reaction kinetics in SCW probed using muonium.

**J.-P. Jay-Gerin (U. of Sherbrooke):** Computational modelling of water radiolysis in high temperature water (including SCW).

**C. Wren (U. of Western Ontario):** Water radiolysis effects on materials degradation in high temperature water (including SCW).

The chemistry program is co-ordinated by D. Guzonas (AECL).

### **3. Activities at the University of New Brunswick (UNB)**

#### **D. H. Lister**

##### ***International Collaboration on “Improved Sample Technique”***

The joint activity with Japan on sampling steam/water systems continued, despite the tragedy in Japan in early 2011 and the withdrawal of the University of Tokyo from the project. UNB took over the CFD simulation of the heat exchanger and sample line attached to their laboratory autoclave, and Dr. Uchida (JAEA) developed the mathematical model to describe the hold-up of corrosion products seen in the UNB experiments. Following the recommendations made at the 2011 meeting of the PCC Working Group in Plsen, several more experiments on sampling from high-temperature water containing iron corrosion products under different temperatures and pHs were undertaken. The CFD simulation was completed and compared with the measurements, and the mathematical model was developed and helped to explain the observations. Presentations on progress were made at this week’s PCC meeting, and a final report has been prepared.

##### ***Complementary Sampling Experiments – Sampling from a Two-Phase Steam-Water System***

In an experimental program looking at flow-accelerated corrosion (FAC) of carbon steel in two-phase steam-water mixtures, a sample system was installed in the high-temperature loop to draw fluid from the wall of a pipe and from the centre flow. Samples of ammoniated fluid taken at various sampling flow rates indicated the kinetics of distribution of the ammonia between liquid and vapour and allowed estimates to be made of the flow regime and the thickness of the liquid film at the wall – important parameters for understanding FAC. The work was described in presentations at this week’s PCC meeting.

##### ***General Research on Chemistry and Corrosion in Power System Coolants***

Research programs continue on the effects of amine additives on FAC in two-phase systems, on developing an in-plant monitor and modelling capabilities for FAC in fossil and nuclear power systems, on determining the kinetics of corrosion-product dissolution in coolant systems, and on the effects of additives on the fouling of heat exchangers in cooling water systems.

#### **W. Cook**

Dr. Cook maintains active research programs related to corrosion and chemistry control in nuclear power reactors and has been very active in the Generation IV International Forum (GIF) through the Canadian National Program. Dr. Cook participated in Phase I of the program and received funding for his Phase II proposal. A major focus is corrosion-product transport and deposition in the core of a SCWR; both experimental techniques and modeling are employed to elucidate material corrosion and the deposition kinetics of the “fall-out” from solution that occurs upon traversing the critical point. The fitting parameters for the R-HKF thermodynamic extrapolation model have been re-examined and applied in the temperature region around the pseudo-critical point. It is believed that electrostatic models such as the R-HKF are applicable in supercritical water (SCW) at moderate temperatures because of the clustering nature of SCW, particularly near a surface, which may allow electric double-layers to persist well beyond the critical transition.



Dr. Cook was on sabbatical leave from UNB, spending four months at Atomic Energy of Canada Limited (AECL) Chalk River Laboratories (CRL) followed by eight months as a technical advisor in the Chemistry Department at the Point Lepreau Nuclear Generation Station; this plant is now being re-started after a prolonged refurbishment outage. During his stay at CRL, he worked closely with Dr. D. Guzonas and the two produced a review article on the link between corrosion and chemistry in a SCWR (“Cycle chemistry and its effect on materials in a supercritical water-cooled reactor: A synthesis of current understanding”, Corrosion Science, 2012).

#### **4. Activities at AECL**

Recent water chemistry work for the Canadian SCWR concept at AECL has focused on studying the relationship between corrosion in relatively high-density SCW (e.g., above the critical temperature at a pressure of 25 MPa) and in ‘superheated steam’ (e.g., low density SCW above the critical temperature but below the critical pressure). The important role played by the solubility of the corrosion films formed on alloy surfaces has been demonstrated in a series of corrosion tests at constant temperature and variable SCW density. With Prof. Cook (UNB), a phenomenological model of the change in corrosion mechanism from electrochemical oxidation in high density SCW to gas-phase (chemical) oxidation in low density SCW was developed. The ability of an alloy surface to impose a local structure on the surface that is different than that in the bulk is currently being studied using a combination of neutron scattering and molecular dynamics modeling.

#### **5. Activities at the University of British Columbia**

##### **R. Pawlowicz**

Activities related to the IAPWS subcommittee on seawater (SCSW):

- 1) Publication of a “history” of TEOS-10. This paper is meant to document the evolution of TEOS-10, and the interactions (both scientific and bureaucratic) between SCOR, IAPSO, IAPWS, and the researchers involved : Pawlowicz, McDougall, Feistel, and Tailleur, An historical perspective on the development of the Thermodynamic Equation of Seawater - 2010, Ocean Sci., 8, 161-174, (2012)
- 2) Numerical modelling of electrical conductivity of seawater at high temperatures and salinities, resulting in a publication: Pawlowicz, The electrical conductivity of seawater at high temperatures and salinities, Desalination 300, 32-39 (2012)
- 3) Numerical modelling of electrical conductivity and density of low-salinity lake and river waters, with the aim of adapting TEOS-10 to those kinds of waters. Publication accepted: Pawlowicz and Feistel, Limnological applications of the Thermodynamic Equation of Seawater 2010 (TEOS-10), Limnology and Oceanography: Methods, in press (accepted June 2012)
- 4) Wrote a peer-reviewed pedagogical article on salinity and heat in the ocean: Pawlowicz, "Key Variables: Temperature, Salinity and Density", online in Physical Oceanography Topic Room, Nature Education Knowledge Project (accepted Aug 2012)
- 5) Began translation of some Chinese-language scientific articles on “Chinese Standard Seawater” the oceanographic conductivity reference material used in China, about which little is known in the west (with assistance of Chuning Wang, a new graduate student from China)
- 6) Developed proposal for 'Joint IAPWS/SCOR/IAPSO Committee on the Properties of Seawater', circulated to both SCOR, IAPSO, and the IAPWS SCSW.

# REPORT

## on IAPWS-related activities: August 2011 – August 2012

submitted by the

**Czech National Committee for the Properties of Water and Steam (CZ NC PWS)**  
to the Executive Committee Meeting of 2012 IAPWS Meeting, Boulder, USA in September 2012

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### *Participating institutions*

The following Czech Institutions have participated in the research of thermophysical properties and chemical processes between August 2011 and August 2012:

**Institute of Thermomechanics AS CR, v. v. i., ("IT ASCR")**, Department of Thermodynamics, Dolejšková 1402/5, CZ-182 00 Praha 8

**Czech Technical University in Prague ("CTU")**, Faculty of Mechanical Engineering, Department of Fluid Mechanics and Thermodynamics, and Department of Power Engineering, Technická 4, CZ-166 07 Praha

**Institute of Chemical Technology Prague ("ICT")**, Power Engineering Department ("ICT-IE") and Department of Physical Chemistry ("ICT-IPC"), Technická 5, CZ-166 28 Praha 6

**University of West Bohemia ("UWB")**, Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitní 8, CZ-306 14 Plzeň

**ŠKODA POWER**, Plzeň, Inc., A Doosan Company, Tylova 57, CZ-316 00 Plzeň

**Technical University of Liberec ("TUL")**, Department of Chemistry, CZ-461 19 Liberec

**SIGMA Research and Development Institute ("SIGMA")**, Jana Sigmunda 79, CZ-783 50 Lutín



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## *Funding*

The activities described below were sponsored by the Grant Agency of the Academy of Sciences of the Czech Republic (GAČR), the Czech Science Foundation (GAČR), ŠKODA POWER, Ministry of Education, Youth and Sport of the Czech Republic (MŠMT), and Ministry of Industry and Trade of the Czech Republic (MPO).




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### *Board of CZ NC PWS for 2010-2013:*

Dr. J. Hrubý  
 Prof. R. Mareš  
 Dr. T. Němec  
 Prof. P. Šafařík  
 Prof. J. Šedlbauer

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### *List of IAPWS-Related Activities*

The Czech Committee in collaboration with the University of West Bohemia organized the 2011 IAPWS Meeting in Plzeň (Pilsen). The Meeting was attended by 24 participants from the Czech Republic and they presented 12 papers [1-12].

Information about new documents adopted and authorized by IAPWS were published on the CZ NC PWS website.

The joint project of IT ASCR and UWB sponsored by the Ministry of Education, Youth and Sports of the Czech Republic provided financial support for international collaboration with IAPWS since 2009. The project support will end on 31/12/2012.

Dr. Hrubý (IT ASCR) and his collaborators studied thermodynamic properties of condensing steam flow, measured density of supercooled water at high pressures, and conducted research into thermodynamic modeling of hydrates of water–carbon dioxide mixtures [1, 8, 13-19].

Prof. Mareš (UWB) and his collaborators studied surface tension of water and other properties of water and steam [3, 20-24].

Prof. Mareš and Dr. Kalová (UWB) in collaboration with Prof. Anisimov (USA) studied thermophysical properties of supercooled water [2, 25-27].

Prof. Maršík (IT ASCR) and his research team studied problems of droplet nucleation in water and the influence of thermophysical properties of water on the efficiency of hydrogen fuel cells [6, 7, 28-30].

Prof. Šedlbauer (TUL) coordinated the IAPWS-IUPAC Joint Project entitled “Establishing recommended data on thermodynamic properties of hydration for selected organic solutes and gases” [4].

The research team at CTU continued to study wet steam energy losses in LP steam turbines (publications are in preparation).

Dr. Sedlář (SIGMA) studied the problems of bubble fission and cavitation instabilities in water turbines and pumps [31-32].

Dr. Jiříček (ICT-IE) and his collaborators studied the problem of renewable power sources and chemical effects in water and steam systems of power plants [33-35].

Dr. Hnědkovský (ICT-IPC) and his collaborators studied the properties of organic solutes in water [36-49].

Prof. Šťastný (ŠKODA POWER) and his co-workers tested and applied a numerical model of steam flow in nozzles and turbine blade cascades with NaCl binary nucleation and condensation [4, 50, 51].

### ***IAPWS Young Scientist Fellowships***

In 2011, **Dr. Vinš** completed his IAPWS Young Scientist Fellowship Project (exchange between the Czech Republic and Germany) entitled “Development of Thermodynamic Models for Hydrates in Water – Carbon Dioxide Mixtures” jointly supervised by Dr. Hrubý and Prof. Span. The preliminary results were presented and discussed during the 2011 IAPWS Meeting in Plzeň [8]. The final Project Report will be presented during the 2012 IAPWS Meeting in Boulder. Five papers and presentations were published [15-19].

**Dr. Holten** is currently completing his IAPWS Young Scientist Fellowship Project (exchange between the Czech Republic and USA) entitled “Towards an IAPWS Guideline for the Thermodynamic Properties of Supercooled Water” jointly supervised by Dr. Hrubý, Prof. Anisimov, and Dr. Sengers. The preliminary results will be presented during the IAPWS Meeting 2012 in Boulder. One journal paper was published [25].

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- 9) Nezbeda, I. : From Ice to Steam and Aqueous Solutions with a Non-Speculative Molecular Model. (A contribution at the 2011 IAPWS Meeting Symposium).
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## German National Committee to IAPWS

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

#### Report "Research in Progress 2012"

**Baltic Sea Research Institute, Warnemuende**

**Dr. Rainer Feistel**

#### Book Publication

Feistel, R., Ebeling, W. (2011): Physics of Self-Organization and Evolution. Wiley-VCH, Weinheim, 517 pp.

#### Articles

Pawlowicz, R., McDougall, T., Feistel, R., Tailleux, R. (2012):  
Preface: An historical perspective on the development of the Thermodynamic Equation of Seawater – 2010.

Ocean Science 8, 161–174, <http://www.ocean-sci.net/8/161/2012/>

Safarov, J., Berndt, S., Millero, F., Feistel, R., Heintz, A., Hassel, E. (2012):  
(p,  $\rho$ , T) properties of seawater: Extensions to high salinities.  
Deep-Sea Research I 65, 146-156

McDougall, T.J., Feistel, R., Pawlowicz, R. (2012):  
Thermodynamics of Seawater.

In: Gerold Siedler, John Church, John Gould, Stephen Griffies (eds.) Ocean Circulation and Climate, second edition, Academic Press (Elsevier), in press

Feistel, R., Wagner, W. (proposers):  
Guideline on a Low-Temperature Extension of the IAPWS-95 Formulation for Water Vapor.  
The International Association for the Properties of Water and Steam, Boulder, Colorado, USA, September/October 2012, to be adopted

Pawlowicz, R., Feistel, R. (2012):  
Limnological applications of the Thermodynamic Equation of Seawater 2010 (TEOS-10).  
Limnology & Oceanography - Methods, submitted

Feistel, R. (2012):  
Thermodynamic Properties of Seawater in Oceanography, [Eds. UNESCO-EOLSS Joint Committee],  
in Encyclopedia of Life Support Systems(EOLSS), Developed under the Auspices of the UNESCO, Eolss Publishers, Oxford, UK, [<http://www.eolss.net>]  
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Feistel, R. (2012):

TEOS-10: A New International Oceanographic Standard for Seawater, Ice, Fluid Water and Humid Air.

International Journal of Thermophysics, DOI: 10.1007/s10765-010-0901-y,  
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Marion, G.M., Millero, F.J., Camoes, F., Spitzer, P., Feistel, R., Chen, C.-T.A. (2011):  
 pH of Seawater.

Marine Chemistry 126, 89–96

Wagner, W., Riethmann, T., Feistel, R., Harvey, A.H. (2011):

New Equations for the Sublimation Pressure and Melting Pressure of H<sub>2</sub>O Ice Ih.

Journal of Physical and Chemical Reference Data, 40, 043103; doi:10.1063/1.3657937 (11 pages)

## **Leibniz Institute for Tropospheric Research, Leipzig**

### **Dr. Olaf Hellmuth**

#### Recent Publications

Hellmuth, O.:

Weather forecast.

In: C. Bernhofer, J. Schanze and J. Seegert: A Textbook on Integrated Flood Risk Management, Springer-Verlag, Berlin (submitted and accepted in 2011).

Hellmuth, O., Khvorostyanov, V. I., Curry, J. A., Shchekin, A.K., Schmelzer, J. W. P., Baidakov V. G. (2011):

Review on the Phenomenology and Mechanism of Atmospheric Ice Formation: Selected Questions of Interest. In: J. W. P. Schmelzer, G. Röpke, and V. B. Priezzhev (eds.): Nucleation Theory and Applications,

JINR Dubna, 483 pp., ISBN 978-5-9539-0301-8, <http://theor.jinr.ru/meetings/2012/nta/>

Hellmuth, O., Khvorostyanov, V. I., Curry, J. A., Shchekin, A.K., Schmelzer, J. W. P., Feistel, R., Djikaev, Y., Baidakov V. G. (2012):

Theoretical Aspects of Atmospheric Ice Formation. In: J. W. P. Schmelzer (eds.): Nucleation Theory and Applications. Special Issues.

Review Series on Selected Topics of Atmospheric Sol Formation, Volume 5, JINR Dubna (textbook, in press).

**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 water and steam in CFD and non-stationary calculations.
- An algorithm for generating spline-interpolation data grids with optimized data density for the user requirements 'range of state' and 'accuracy' was developed.

**2. Stoffwerte für Wasser und Wasserdampf (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, is being worked on. The reference for this publication will read: *Wagner, W. and Kretzschmar, H.-J.*, Stoffwerte von Wasser und Wasserdampf, VDI-Wärmeatlas, 11. Auflage, Abschnitt D2.1, pp. 1-15, Springer-Verlag, Berlin. Status: The proofs are being checked.

**3. Property Libraries for Calculating Heat Cycles**

- The property library LibIF97 for steam and water has been extended to ice properties including sublimation and melting pressures.
- The property libraries for steam, water, ice, seawater, humid combustion gases, humid air, ammonia/water mixtures and water/lithium bromide mixtures have been connected to LabVIEW.
- An Online Property Calculator for calculating thermodynamic and transport properties for steam, water and other working fluids in power engineering was installed on the website [www.thermodynamics-zittau.com](http://www.thermodynamics-zittau.com).
- A steam tables App for iPhone, iPad, and iPod touch has been developed.
- A student version of the steam tables program FluidLAB for MATLAB was prepared and its link installed on the IAPWS Website [www.iapws.org](http://www.iapws.org) under "Education".

**Recent Publications**

Kretzschmar, H.-J., Kraft, I.:  
Kleine Formelsammlung Technische Thermodynamik, 4. Auflage.  
Carl Hanser Verlag, München (2011)

Kretzschmar, H.-J.:  
Bereitstellung von thermodynamischen Stoffdaten für Arbeitsfluide der Energietechnik.  
In: Aktuelle Beiträge zur Technischen Thermodynamik, Energietechnik und

Fernwärmeversorgung,  
Verlag AGFW, Frankfurt am Main (2011)

Herrmann, S.; Kretzschmar, H.-J.; Gattley, D. P.:  
Berechnung der thermodynamischen Eigenschaften von feuchter Luft.  
KI - Kälte Luft Klimatechnik, 48 (2012) S. 22-28

Kunick, M; Kretzschmar, H.-J.; Gampe, U.:  
Schnelle und flexible Berechnung thermodynamischer Stoffwerte mit Spline-Interpolation für  
die Modellierung instationärer Energieumwandlungsprozesse.  
In: W. Honekamp, P. Schindler, Tagungsband der 13. Nachwuchswissenschaftlerkonferenz  
mitteleuropäischer Fachhochschulen Görlitz, S.209-214, Re Di Roma-Verlag, Remscheid (2012),  
ISBN 978-3-86870-436-5

Kretzschmar, H.-J., Stöcker, I.:  
*Mollier h,s-Diagramm von Wasserdampf (Mollier h-s Diagram for Steam).*  
Siemens Energy, Erlangen (2012)

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

**Projects**

The group chaired by Prof. Span has actively been involved in a number of research projects related to CO<sub>2</sub>-rich mixtures as they are typical for power generation with carbon capture and storage (CCS). On its 2011 meeting IAPWS has encouraged this kind of work under ICRN 27, *Thermodynamic Properties of Humid Gases and CO<sub>2</sub>-Rich Mixtures*. The work of Prof. Span primarily addresses the

- improvement of the experimental data base available for CCS-relevant mixtures. As part of this activity co-operations with colleagues at the University of Valladolid and at SINTEF in Trondheim were established.
- improvement of accurate models available for CCS-relevant mixtures. Main foci of this work have been the development of improved mixing models and a consistent description of complex phase equilibria, 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 (Hruby and Vins, see separate report presented by Dr. Vins) and with Dr. E. W. Lemmon at NIST in Boulder.
- application of accurate property models in process simulation. The relevance of the accuracy of property models could be shown both for the processes of the LNG product-chain and for CCS-applications.

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 scope of IAPWS.

## Journal Articles and Proceedings

- F. Dauber, J. Gernert, R. Span and P. Schley:  
On the Use of Highly Accurate Thermodynamic Property Models in Process Simulation.  
Proceedings International Gas Union Research Conference - IGRC, Seoul (2011).
- R. Span:  
Kraftwerkstechnik mit CO<sub>2</sub>-Rückhaltung – Anforderungen an Stoffdatenmodelle.  
In: Nordrhein-Westfälische Akademie der Wissenschaften und Künste, Ferdinand Schöningh Verlag, Paderborn, ISBN 978-3-506-77367-8 (2011).
- M. E Mondéjar, M. C. Martín, R. Span and C. R. Chamorro:  
New ( $p, \rho, T$ ) data for carbon dioxide - nitrogen mixtures from 250 K to 400 K at pressures up to 20 MPa.  
J. Chem. Thermodynamics 43, 1950–1953 (2011).
- M. E Mondéjar, M. C. Martín, R. Span and C. R. Chamorro:  
( $p, \rho, T$ ) behavior of two mixtures of carbon monoxide with nitrogen in the temperature range from 250 K to 400 K and pressures up to 20 MPa.  
J. Chem. Eng. Data 56, 3933–3939 (2011).
- V. Vins, A. Jäger, J. Hrubý and R. Span:  
Phase equilibria of carbon dioxide and methane gas-hydrates predicted with the modified analytical S-L-V equation of state.  
Proc. Experimental Fluid Mechanics, Czech Republic (2011).
- M. E. Mondéjar, R. M. Villamañán, R. Span, and C. R. Chamorro:  
Accurate ( $p, \rho, T$ ) data for two new (carbon dioxide+nitrogen) mixtures from (250 to 400)K at pressures up to 20MPa.  
J. Chem. Thermodyn. 48, 254–259 (2012)
- A. Jäger and R. Span:  
Equation of state for solid carbon dioxide based on the Gibbs free enthalpy.  
J. Chem. Eng. Data 57, 590-597 (2012)

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

## Projects

1. Stoffwerte für Wasser und Wasserdampf (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, is being worked on. The corresponding steam tables are calculated based on the Industrial Formulation IAPWS-IF97 and the current equations for the transport properties and other properties based on the

corresponding IAPWS Releases. The reference for this publication will read: *Wagner, W. and Kretzschmar, H.-J.*, Stoffwerte von Wasser und Wasserdampf, VDI-Wärmeatlas, 11. Auflage, Abschnitt D2.1, pp. 1-15, Springer-Verlag, Berlin. Status: The proofs are being checked.

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).

Current Status of Research Activities in Japan

**Submitted to the Executive Committee Meeting, IAPWS,  
Bolder, Colorado, USA, September 2012**

by

Japanese National Committee  
International Association for the Properties of Water and Steam  
c/o The 139<sup>th</sup> Committee on Steam Properties  
Japan Society for the Promotion of Science (JSPS)  
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Recent Publications:

Shunsuke Uchida, PhD,

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- [2] Naitoh, M., Uchida, S., Okada, H., and Koshizuka, S., "Validation of Code System DRAWTHREE-FAC for Evaluation of Wall Thinning due to Flow Accelerated Corrosion by PWR Feed Water Piping Analysis", Proc. ASME 2011 Pressure Vessel & Piping Division Conference, PVP2011, July 17-21, 2011, Baltimore, Maryland, USA, American Society of Mechanical Engineers, PVP2011- 57120 (2011).
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- [7] Uchida, S., Naitoh, M., Okada, H., Ohira, T., Koshizuka, S., and Lister, D. H., "Verification and Validation of Evaluation Procedures for Local Wall Thinning due to Flow Accelerated Corrosion and Liquid Droplet Impingement", Nucl. Technol., 178, 280 (2012).
- [8] Uchida, S., Asakura, Y., and Suzuki, H., "Deposition of Boron on Fuel Rod Surface under Sub-cooled Boiling Conditions - An Approach toward Understanding AOA Occurrence", Nucl. Eng. Design, 241, 2398-2410 (2011).
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- [10] Uchida, S., Naitoh, M., Okada, H., and Suzuki, H., "Water Chemistry Guidance in Nuclear Power Plants in Japan", Nucl. Eng. Int., December, 30-31 (2011).
- [11] Uchida, S., Naitoh, M., Okada, H., and Suzuki, H., "Water Chemistry Guidance in Nuclear Power Plants in Japan", Power Plant Chemistry, 14 (1), 5-17 (2012)

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URL: <http://www.tagen.tohoku.ac.jp/labo/muramatsu/index.html>

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URL: <http://www.tagen.tohoku.ac.jp/modules/laboratory/index.php?laboid=49>

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## International Association for the Properties of Water and Steam Russian National Committee (RNC)

### Report Second Half-Year of 2011- First Half-Year of 2012

1. RNC active participation in organization of 5-th International Water-Chemistry Forum, April 2012, Moscow, MPEI.
2. Three meetings of RNC have been held. Current problems are investigated.

#### Publications list

1. T. Petrova, V. Voronov, B. Larin. Technology of the water chemistry of nuclear power plants. Moscow, MPEI Publishing House, 2012 (text book).
2. A. Panteleev, B. Ryabchikov, O. Khoruzhii, S. Gromov, A. Sidorov. Membrane Technologies in the Industrial Water Treatment. Moscow. Deli Plus, 2012 (text book).
3. A. Alexandrov, E. Dzhuraeva, and V. Utenkov. Viscosity of Aqueous Solutions of Sodium Chloride. High Temperature, 2012, Vol. 50, No. 3, pp. 354–358
4. A. Alexandrov, E. Dzhuraeva, and V. Utenkov. Dynamic viscosity of aqueous solutions of sodium sulfate. Proceedings of the National Conference "Improving the efficiency, reliability and safety of power equipment on thermal and nuclear power plants". Moscow, MPEI, April 4-6, 2012.
5. V. Ochkov. Water and Magnet // Water Purification, Water Treatment, Water Supply, # 10, 2011, pp. 36-48.
6. V. Ochkov "Cloud" Service on the Properties of Working Media for Thermal Engineering Calculations. Thermal Engineering, #07, 2012, pp. 566-572.
7. V. Ochkov F., K. Orlov. Cloud-computing Functions for Thermodynamic Properties Calculation // Symposium on thermophysical properties of Fluids, September 14, 2012 in Zittau, Germany.
8. K. Orlov. Thermal properties calculation using GPU computing // Eighteenth Symposium on Thermophysical Properties, National Institute of Standards and Technology, Boulder, USA, June 24 - 29, 2012.
9. K. Orlov Criteria for competitive analysis. 5-th International Water-Chemistry Forum, April 2012, Moscow, MPEI.
10. T. Petrova. I. Burakov. The corrosion rate of carbon steel in boiling water containing a film-forming amines at elevated concentrations of NaOH. Novoe v rossiyskoy elektroenergetike (New in Russian elektroenergetiks), #12, 2011, pp. 7-13.
11. T. Petrova. I. Burakov. The use of film-forming amines on the TPP with drum boilers and waste heat boilers. Proceedings of the 2nd All-Russian Conference "Improving the safety and operational efficiency of power plants and power systems". Moscow, MPEI, 4-6 of June, 2012, pp. 235-237.
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15. V. Voronov, O. Egoshina, M. Nazarenko, S. Kolyshnitsina. Operating experience of Chemical Technology Monitoring System in launching mode for unit № 8 PSU 420 of CHP-26 Mosenergo. Proceedings of the National Conference "Improving the efficiency, reliability and safety of power equipment on thermal and nuclear power plants". Moscow, MPEI, April 4-6, 2012.
16. S. Gavrilenko, V. Ochkov. Integrated application of membrane water treatment technologies in the energy sector on the example of the Adler CHP. Proceedings of the National Conference "Improving the efficiency, reliability and safety of power equipment on thermal and nuclear power plants". Moscow, MPEI, April 4-6, 2012.
17. P. Gotovcev, O. Egoshina. Identifying the reasons of water chemistry violations using mathematical modeling. Proceedings of the National Conference "Improving the efficiency, reliability and safety of power equipment on thermal and nuclear power plants". Moscow, MPEI, April 4-6, 2012.
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22. V. Vinogradov, A. Larin Use of Oxygen Measurement Techniques for Estimating the Intensity of Microbiological Processes and Inhibiting Them in Water Treatment Plants. *Thermal Engineering*, #07, 2012, pp. 513-516.
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37. V. Ochkov, V. Voloshchuk. Modern information technology for power system: cloud features on the properties of working fluids, calculation cycle steam turbine, gas turbine, combined cycle gas turbines and heat pumps // Proceedings of the 7th International Scientific Conference "Modern problems of refrigeration equipment and technology", Odessa, Ukraine 14-16 of September, 2011, pp. 27-29.
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44. P. Gotovcev, Khizova E. I. Municipal water supply system and waste water systems. *Proceedings of All-Russian conference "Energy Available" Kislovodsk. 2011.*

## U.S. National Committee to IAPWS 2012 Report on Activities of Potential Interest to IAPWS

**Communicated from the National Institute of Standards and Technology, Boulder, CO and Gaithersburg, MD:**

In collaboration with researchers in Greece and Germany and at the University of Maryland, a new formulation has been developed for the thermal conductivity of water and steam. The complete correlation, which covers a wider range of conditions than the previous formulation and is consistent with IAPWS-95 and the new IAPWS viscosity correlation, has now been adopted by IAPWS and has been published.

Reference: M.L. Huber, R.A. Perkins, D.G. Friend, J.V. Sengers, M.J. Assael, I.N. Metaxa, K. Miyagawa, R. Hellmann, and E. Vogel, New International Formulation for the Thermal Conductivity of H<sub>2</sub>O, *J. Phys. Chem. Ref. Data* **41**, 033102 (2012).

In a collaboration with the Kazan State Technological University (Russia) and the Dagestan Scientific Center of the Russian Academy of Sciences (as part of an IAPWS Collaborative Project), the thermal conductivity of binary ammonia+water mixtures was measured over the temperature range from 278 K to 356 K and at pressures up to 20 MPa using the steady-state hot-wire method. Measurements were made for eight compositions over the entire concentration range. Temperature, pressure, density, and concentration dependences of the thermal conductivity of the mixture were studied. Various types of wide-ranging correlation models for the thermal conductivity of these mixtures were also developed using the measured data.

In NIST's Sensor Science Division (Gaithersburg, MD), a gravimetric apparatus has been constructed for measuring the saturation concentration of water as a function of temperature and pressure in compressed gaseous carbon dioxide (equivalent to a dew-point measurement) at pressures up to 6 MPa and temperatures up to 85 °C. Preliminary results with air (which has been studied previously in other apparatus) validate the reliability of the apparatus, and experiments with CO<sub>2</sub> are currently underway.

In collaboration with NIST's Sensor Science Division, a combined experimental and theoretical study was performed of the effect of atmospheric pressure on the ice point of water, which is used in thermometry. Experiment and theory agreed, confirming results for the sea-level ice point dating to the mid-1900s and for the first time providing a validated method for adjusting the ice point for work at higher elevations.

Reference: A.H. Harvey, M.O. McLinden, and W.L. Tew, Thermodynamic Analysis and Experimental Study of the Effect of Atmospheric Pressure on the Ice Point, *Proceedings of the 9<sup>th</sup> International Temperature Symposium*, in press (2012).

In NIST's Chemical and Biochemical Reference Data Division (Gaithersburg, MD), the vapor pressure of ice has been measured over the temperature range 173 K to 273 K using cavity ring-down spectroscopy to probe the output of a humidity generator which contains isothermal samples of ice in a nitrogen atmosphere. The measurement is relative to the known triple-point pressure, and is corrected for the enhancement factor. Preliminary analysis indicates good agreement with the new IAPWS formulation for the sublimation pressure.

Reference: K. Bielska, D.K. Havey, G.E. Scace, D. Lisak, and J.T. Hodges, Spectroscopic Measurement of the Vapour Pressure of Ice, *Phil. Trans. Royal Soc. A* **370**, 2509 (2012).

### Communicated from the University of Maryland

The research on the thermodynamic behavior of supercooled water was continued, yielding the following publications (supported in part by IAPWS):

1. V. Holten, C.E. Bertrand, M.A. Anisimov, and J.V. Sengers, "Thermodynamics of supercooled water, J. Chem. Phys. **136**, 0945507 (2012).
2. V. Holten, J. Kalová, M.A. Anisimov, and J.V. Sengers, "Thermodynamics of liquid-liquid criticality in supercooled water in a mean-field approximation", Int. J. Thermophys. **33**, 758-773 (2012).

In addition, a new updated equation was developed for the critical locus of aqueous solutions of NaCl:

3. D.A. Fuentesvilla, J.V. Sengers, and M.A. Anisimov, "Critical locus of aqueous solutions of sodium chloride revisited", Int. J. Thermophys. **33**, 943-958 (2012).

A draft of a new guideline on the critical locus of aqueous solutions was prepared for IAPWS.

### Communicated from Andre Anderko, OLI Systems

In 2011-2012, the work at OLI Systems was focused on the following projects:

- (1) A previously developed comprehensive model for thermal conductivity of electrolyte solutions has been revised by using the new IAPWS formulation for the thermal conductivity of pure water. The application of this model to seawater has been explored in detail and the results have been published. In the near future, we are planning to create an IAPWS guideline for the thermal conductivity of seawater based on this model.

Reference: P. Wang and A. Anderko, "Modeling Thermal Conductivity of Electrolyte Mixtures in Wide Temperature and Pressure Ranges: Seawater and Its Main Components", *Int. J. Thermophysics*, **33** (2012) 235-258.

- (2) In collaboration with the Pacific Northwest National Laboratory, work was continued on modeling the behavior of systems containing carbon dioxide, water, and various salts. This work encompasses the behavior of both water-rich and CO<sub>2</sub>-rich phases. Also, implications for mineral reaction equilibria have been explored.

Reference: R.D. Springer, Z. Wang, A. Anderko, P. Wang, and A.R. Felmy, "A Thermodynamic Model for Predicting Mineral Reactivity in Supercritical Carbon Dioxide: I. Phase Behavior of Carbon Dioxide – Water – Chloride Salt Systems Across the H<sub>2</sub>O-Rich to the CO<sub>2</sub>-Rich Regions", *Chemical Geology*, **322-323** (2012) 151-171.

- (3) A comprehensive model has been developed for predicting the phase equilibria of selected actinides (i.e., U, Pu, and Am) in aqueous systems. This includes the behavior of oxides and hydroxides in wide ranges of temperature, pH, and salinity and the behavior of actinides in concentrated acid solutions.
- (4) An electrochemical model has been developed for predicting general and localized corrosion of the copper-nickel alloy CuNi7030. This work extends our previous work on the corrosion behavior of copper-nickel alloys.
- (5) Work was continued on developing a model for predicting interfacial tension.