

The Czech National Committee
International Association for the Properties of Water and Steam

REPORT on IAPWS related activities – July 2010 / August 2011

Submitted to the EC Meeting of IAPWS, Plzeň, Czech Republic – September 2011.

National Committee Contacts:

CZ NC PWS, Institute of Thermomechanics AS CR, v.v.i., Dolejškova 5, 182 00 Prague 8,
Czech Republic, Fax: + 420 2858 4695, E-mail: secr.czncpws@it.cas.cz
Head: Dr. Jan Hruby, E-mail: hruby@it.cas.cz

Following Institutions participated in the research into the thermophysical properties and in chemical processes:

Institute of Thermomechanics (IT) AS CR, v.v.i., Department of Thermodynamics, Dolejskova 5, CZ-182 00 Prague 8.

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

Institute of Chemical Technology Prague (ICT), Power Engineering Department (ICT-IE) and Department of Physical Chemistry (ICT-IPC), Technicka 5, CZ-166 28 Prague 6.

University of West Bohemia (UWB), Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitni 8, CZ-306 14 Plzen.

SKODA POWER, Plzen, Inc., Tylova 57, CZ-316 00 Plzen.

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

SIGMA Research and Development Institute (SIGMA), Jana Sigmunda 79, CZ-783 50 Lutin.

Activities were sponsored by the Grant Agency of the Academy of Sciences of the Czech Republic, Grant Agency of the Czech Republic, SKODA POWER Plzen, Ministry of Education, Youth and Sport of the Czech Republic, and Ministry of Industry and Trade of the Czech Republic.

The board of the CZ NC PWS for the period 2010-2013:

Dr. J. Hruby, Prof. R. Mares, Dr. T. Nemeč, Prof. P. Safarik, and Prof. J. Sedlbauer.

- In the 2010 IAPWS Meeting in Niagara Falls, Canada participated 7 workers from CzR. One of presented papers is in Ref. [1].
- Brief information has been published on web sites of CZ NC PWS to the new documents adopted and authorized by IAPWS.
- A joint project IT AV ČR and WBU Plzen sponsored by the Ministry of Education, Youth and Sports (MEYS, MŠMT in Czech) enables cooperation with IAPWS for the next two years, till 2012 inclusive.
- Dr. Hruby (IT) with his collaborators investigated properties of homogeneous and heterogeneous nucleation and heat transfer, Refs. [2 to 6].
- Prof. Mares (UWB) with his collaborator investigated a temperature dependence of the surface tension of water, Refs [7 and 8]
- Prof. Mares and Dr. Kalova (UWB) collaborated with Prof. M. A. Anisimov (USA) and investigated thermophysical properties of supercooled water, Ref.[9]

- Prof. Marsik (IT) with his research team studied condensation problems and cavitations processes, Refs. [1, and 10 to 12].
- Prof. Sedlbauer (TUL) and his team continued in the research into chemistry of aqueous systems. Refs. [13 and 14]
- Prof. Sedlbauer (TUL) coordinated IAPWS-IUPAC Joint Project: Establishing recommended data on thermodynamic properties of hydration for selected organic solutes and gases.
- Research activities at the (CTU) continued in further improvement of the current knowledge on the following subjects: determination of the heterogeneous particles in the superheated steam in turbines, Ref. [2], and development of correction in classical nucleation theory, Ref. [15].
- The problems studied in SIGMA Research and Development Institute (SIGMA) have been related mainly to the problems of nucleation processes and bubble dynamics during hydrodynamic cavitation and problems of cavitation instabilities in hydraulic machinery. Refs. [1 and 16].
- Dr. Jiricek (ICT-IE) with collaborators investigated renewable power sources and chemical effects in water and steam systems of power plants. Refs. [2, 17 to 21].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are under Refs. [22 and 37].
- Prof. Stastny (SKODA POWER) with co-workers tested and applied the numerical model of the steam flow in nozzles and turbine blade cascades with NaCl binary nucleation and condensation, Ref. [38].
- ICT-IE organized 8th International Conference on Power Cycle Chemistry (CHEO8) from 7th to 8th September 2010 in Prague.
- Dr. Nemeč worked with Dr. A. Harvey (USA) on some improvements to the IAPWS website that will increase the usability of the website.
- The CZ NC PWS collaborated with IT and WBU on the preparation and organization of the IAPWS Meeting 2011, Plzeň.

Young Scientists IAPWS Fellowships

Information on the Young Scientists IAPWS Fellowship Projects.

- Dr. V. Vins performs his Young Scientist IAPWS Fellowship Project (CZ-Germany) "Development of Thermodynamic Models for Hydrates in Water – Carbon Dioxide Mixtures" under supervising of Dr. J. Hruby and Prof. R. Span. Preliminary results will be presented and discussed at the 2011 IAPWS Meeting in Plzeň. The Final Report of the Project will be finished by the end of the year 2011.
- Dr. Kalova handed over the Final Report finished in the frame of the Young Scientists IAPWS Fellowship Project 2010 „Thermophysical Properties of Supercooled Water”. A brief summary will be presented on negotiations of WG PCAS at the IAPWS Meeting 2011 in Plzeň. The results will be published in proceedings and journals.

References:

- [1] Sedlar M., Nemeč T. and Marsik F.: Homogenous Nucleation During Cavitation Processes and Its Modelling by CFD, Presentation IAPWS Annual Meeting 2010, Niagara Falls, 2010.
- [2] Hruby J., Kolovratnik M., Zdimal V., Bartos O., Moravec P., Jiricek I.: Nonequilibrium Condensation Processes in Steam Turbines in the Light of New

- Measurements of Heterogeneous Particles, pp.45-52. In: Proceedings of the 9th Conference on Power System Engineering, Thermodynamics & Fluid Flow (ES 2010), Pilsen, 2010.
- [3] Novak A., Hruby J., Kozel K.: Boiling Two Phase Flow in a Coil-Shaped Duct Combined with Heat Conduction in Solid Body, pp.795-804. In: Proceedings of the International Conference Experimental Fluid Mechanics 2010, Liberec, 2010.
- [4] Peukert P., Hruby J.: Measurement of Heat Transfer on an Experimental Exchanger with a Specially-Shaped Capillary Tube, pp.105-110 (in Czech). In: Proceedings of the 9th Conference on Power System Engineering, Thermodynamics & Fluid Flow (ES 2010), Pilsen, 2010.
- [5] Peukert P., Hruby J.: Results of Measurements at a Laboratory Condensation Heat Exchanger with a Corrugated Minichannel Tube, pp.515-523. In: Proceedings of the International Conference Experimental Fluid Mechanics 2010, Liberec, 2010.
- [6] Vins V., Hruby J., Plankova B.: Droplet and Bubble Nucleation Modeled by Density Gradient Theory - Cubic Equation of State versus SAFT Model, pp.795-804. In: Proceedings of the International Conference Experimental Fluid Mechanics 2010, Liberec, 2010.
- [7] Kalova J., Mares R.: Temperature Dependence of the Surface Tension of Water, In: Proceedings of the 10th conference on Power System Engineering, Thermodynamics & Fluid Flow - ES 2011, Pilsen, 2011. (in Czech)
- [8] Kalova J., Mares R.: Dependence of the Surface Tension on a Geometric Shape of the Phase Interface, pp.81-84. (in Czech) In: Proceedings of the 30th Meeting of Fluid Mechanics and Thermomechanics Departments, Spindleruv Mlyn, 2011
- [9] Kalova J., Mares R., Anisimov M.A.: Thermophysical Properties of Supercooled Water, Report for the Young Scientists IAPWS Fellowship, Pilsen, 2011
- [10] Nemec T., Marsik F.: Classical Nucleation Theory for Cavitation Processes in Water, pp.2035-2040. In: Proceedings of the 7th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics (HEFAT2010). Antalya, 2010.
- [11] Nemec T.: Nucleation Rate in Binary Cavitating Systems - A Comparison of Experimental Data and Classical Nucleation Theory Predictions pp.439-451. In: International Conference Experimental Fluid Mechanics 2010. Conference Proceedings Volume 2. Liberec, 2010.
- [12] Nemec T., Marsik F.: Surface Tension in the Classical Nucleation Theory. In: International Aerosol Conference 2010. Helsinki, 2010.
- [13] Sedlbauer J.: Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes and Gases. In: 20th International Conference on Physical Organic Chemistry, Busan, 2010.
- [14] Sedlbauer J., Slavik M.: Establishing Recommended Data on Thermodynamic Properties of Hydration. In: 14th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Leoben, 2010.

- [15] Petr, V., Kolovratnik M.: Classical Nucleation Theory as an Adequate Model in Predicting Related Wet Steam Effects in LP Steam Turbines, pp.991-1002. In: Proceedings of 9th European Conference on Turbomachinery, Fluid Dynamics and Thermodynamics, Istanbul, 2011.
- [16] Sedlar M., Sputa O., Komarek M.: Numerical Modelling of Cavitation Properties of Mixed-Flow Pump. In: Proceedings of the WIMRC 3rd International Cavitation Forum 2011, Warwick, 2011.
- [17] Zemlova T., Jiricek I., Janda V.: Organic PCM's for Domestic Hot Water Heating, pp. 140-143. In: Proceedings of CHEO8 Conference, Prague, 2010. (in Czech)
- [18] Jiricek I., Zemlova T., Janda V.: Mixed Fuels Based on Straw, pp.125-129. In: Proceedings of CHEO8 Conference, Prague, 2010. (in Czech)
- [19] Jiricek I., Rudasov, P., Vosejпка J.: Consequences of the Increased Alkalinity in Heating Plant Cycle, pp.80-85. In: Proceedings of CHEO8 Conference, Prague, 2010. (in Czech)
- [20] Zemlova T., Jiricek I., Janda V.: Materials for Heat Storage from Biomass Combustion, pp.142-147. In: Proceedings of Power Engineering and Biomass 2010 Conference, Prague, 2010. (in Czech)
- [21] Jiricek I., Zemlova T., Janda V.: Additivation to Improve Thermal Behaviour of Straw, pp.8-13. In: Proceedings of Power Engineering and Biomass 2010 Conference, Prague, 2010). (in Czech)
- [22] Cibulka I., Hnedkovsky L., Sedlbauer J.: Partial Molar Volumes of Organic Solutes in Water. XX. Glycine(aq) and L-Alanine(aq) at Temperatures (298 to 443) K and at Pressures up to 30 MPa, Journal of Chemical Thermodynamics, Vol.42, No.2, 2010, pp.198-207.
- [23] Cibulka I. Simurka L., Hnedkovsky L : Partial Molar Volumes of Cyclic Ketones at Infinite Dilution in Water at Temperatures $T = (278 \text{ to } 373) \text{ K}$ and Low Pressure, Journal of Chemical and Engineering Data, Vol.55, No.12, 2010, pp.5429-5434.
- [24] Hnedkovsky L., Konigsberger E., Konigsberger L.-C., Cibulka I., Schrodle S., May P.M., Heffer G. : Densities of Concentrated Alkaline Aluminate Solutions at Temperatures from (323 to 573) K and 10 MPa Pressure, Journal of Chemical and Engineering Data, Vol.55, No.3, 2010, pp.1173-1178.
- [25] Cibulka I.: Partial Molar Volumes of Organic Solutes in Water. XXII. Cyclic Ethers at Temperatures (298 to 573) K and Pressures up to 30 MPa, Journal of Chemical Thermodynamics, Vol.42, No.4, 2010, pp.502-512.
- [26] Cibulka I., Alexiou, C.: Partial molar volumes of organic solutes in water. XXI: Cyclic ethers at temperatures $T = (278 \text{ to } 373) \text{ K}$ and at low pressure, Journal of Chemical Thermodynamics, Vol.42, No.2. 2010, pp.274-285
- [27] Dohnal V., Vrbka P., Rehak K., Bohme A., Paschke A.: Activity Coefficients and Partial Molar Excess Enthalpies at Infinite Dilution for Four Esters in Water, Fluid Phase Equilibria, Vol.295, No.2, 2010, pp.194-200
- [28] Ondo D., Dohnal V.: Limiting Activity Coefficients of 1-Chlorobutane in Water and in Aqueous Solutions of Substances Involved in Synthesis of Ionic Liquids, Fluid Phase Equilibria, Vol.299, No.2, 2010, pp.266-271.

- [29] Rak J., Ondo D., Tkadlecova M., Dohnal V.: On the Interaction of Ionic Liquid 1-Butyl-3-Methylimidazolium Hexafluorophosphate with beta-Cyclodextrin in Aqueous Solutions, *International Journal of Research in Physical Chemistry and Chemical Physics*, Vol.224, No.6, 2010, pp.893-906.
- [30] Fenclova D., Dohnal V., Vrbka P., Rehak K.: Temperature Dependence of Limiting Activity Coefficients, Henry's Law Constants, and Related Infinite Dilution Properties of Branched Pentanols in Water. Measurement, Critical Compilation, Correlation, and Recommended Data, *Journal of Chemical and Engineering data*, Vol.55, No.9, 2010, pp.3032-3043.
- [31] Vonka P., Hubkova M., Meistr V.: Calculation of Water Content in Water-Methane System, *Collection of Czechoslovak Chemical Communications*, Vol.75, No.3, 2010, pp.257-274.
- [32] Kolafa J., Oncak M.: Hydrogen-Bond Defect in the Structure of Ice Ih, *Journal of Physical Chemistry*, Vol.114, No.48, 2010, pp.20518-20522.
- [33] Matas K., Kolafa J.: Molecular Dynamics Simulations of Aqueous Solutions of Ionic Liquids, *Collection of Czechoslovak Chemical Communications*, Vol.75, No.3, 2010, pp.333-348
- [34] Forck R.M., Dauster I., Schieweck Y., Zeuch T., Buck U., Oncak M., Slavicek P.: Communications: Observation of Two Classes of Isomers of Hydrated Electrons in Sodium-Water Clusters, *Journal of Chemical Physics*, Vol.132, No.22, 2010, Article No: 221102.
- [35] Oncak M., Lischka H., Slavicek P.: Photostability and Solvation: Photodynamics of Microsolvated Zwitterionic Glycine, *Physical Chemistry Chemical Physics*, Vol.12, No.19, 2010, pp.4906-4914.
- [36] Heyda J., Lund M., Oncak M., Slavicek P., Jungwirth P.: Reversal of Hofmeister Ordering for Pairing of NH₄⁺ vs Alkylated Ammonium Cations with Halide Anions in Water, *Journal of Physical Chemistry B*, Vol.114, No.33, 2010, pp.10843-10852.
- [37] Oncak M., Schroder D., Slavicek P.: Theoretical Study of the Microhydration of Mononuclear and Dinuclear Uranium (VI) Species Derived from Solvolysis of Uranyl Nitrate in Water, *Journal of Computational Chemistry*, Vol.31, No.12, 2010, pp.2294-2306.
- [38] Stastny M., Strasak P.: Wet Steam Flow in Elbow of Pipeline in Nuclear Power Plant. In: *Proceedings of 26th Conference on Computational Mechanics*, WBU, Nectiny, 2010