

Current Status of Research Activities in Japan **Submitted to the Executive Committee Meeting, IAPWS,** **Dresden, Germany, September 2016**

Japanese National Committee, Chaired by Professor Masaru Nakahara
 International Association for the Properties of Water and Steam
 c/o The 139th Committee on Steam Properties
 Japan Society for the Promotion of Science (JSPS)
 5-3-1, Kojimachi, Chiyoda-ku
 Tokyo 102-0083, Japan

I. Overview:

Recently we focus on the contribution to the activities of IAPWS for the development of such documents as the TGD guidance, guidelines, releases etc. Also our efforts are directed to the effective distribution and bilingual availability of the internationally standardized references among our colleagues. Some fundamental research activities on water and aqueous systems, relevant closely or in future to IAPWS, are actively carried out all over our country as can be seen in the publication list below. They can be characterized by key words, such as water, hydrothermal, solvothermal, solvation, interfacial, organic, ionic, and reactions. Some of them are presented by our colleagues in the IAPWS annual meeting in Dresden, Germany. We often hold the national meeting to exchange a wide range of information on the science and technology related to power generation. Industrial and academic people are collaborating in a stimulating manner to seek the present or future problems. Our members cover a variety of IAPWS-related areas and make efforts to seriously consider the improvement of our power cycle systems and operation and safety engineering including the outlet gas treatment to avoid the public nuisance such as air/water/soil pollution. One of the J-Power members, JPE, has been developing “Regenerative Activated Coke Technology” as one of the eminent front runners. Now we are preparing the coming meeting of IAPWS 2017 in Kyoto.

II. Recent Publications:

Nakahara, Masaru

Professor Emeritus of Kyoto University, Institute for Chemical Research
 email: nakahara@scl.kyoto-u.ac.jp

- [1] Nakahara, M.; Yoshida K.; “Chronological Scientific Tables 2016”, pp.502-509, 514-517, Maruzen Publishing Co., Ltd., Tokyo, ISBN 978-4621089651 (2015).
- [2] Yoshida, K.; Matubayasi, N.; Nakahara, M.; Uosaki, Y.; “Effect of Rotation on Vibrational Spectrum of Supercritical Water: Analysis of Dependencies on Density and Hydrogen Isotopes”, *The Review of High Pressure Science and Technology*, **26**, in press (2016).

Hirano, Hideo

Retired Senior Research Scientist, Central Research Institute of Electric Power Industry,

e-mail: hhirano0879@jcom.home.ne.jp

- [1] Hirano, H. “ The Outline of the Revision of JIS B8223 Water conditioning for boiler feed water and boiler water ”, **THE THERMAL AND NUCLEAR POWER**, 67(3), pp. 196-202 (2016).
- [2] Hirano, H. “The Main Revision Points of JIS B 8223 Water conditioning for boiler feed water and boiler water ” , **JOURNAL OF JAPAN BOILER ASSOCIATION**, 398(8), pp. 10-17 (2016).

Yoshida, Ken

Associate Professor, Department of Chemical Science and Technology, Faculty of Engineering, Tokushima University

email: yoshida.ken@tokushima-u.ac.jp

URL: <http://pub2.db.tokushima-u.ac.jp/ERD/person/189117/work-en.html>

- [1] Nakahara, M.; Yoshida K.; “Chronological Scientific Tables 2016”, pp.502-509, 514-517, Maruzen Publishing Co., Ltd., Tokyo, ISBN 978-4621089651 (2015).
- [2] Yoshida, K.; Matubayasi, N.; Nakahara, M.; Uosaki, Y.; “Effect of Rotation on Vibrational Spectrum of Supercritical Water: Analysis of Dependencies on Density and Hydrogen Isotopes”, *The Review of High Pressure Science and Technology*, **26**, in press (2016).

Okazaki, Susumu

Professor, Department of Applied Chemistry, Nagoya University

email: okazaki@apchem.nagoya-u.ac.jp,

URL: <http://simulo.apchem.nagoya-u.ac.jp/index.html>

- [1] Yoshii, N.; Fujimoto, K.; Okazaki, S. “Molecular dynamics study of the structure of anionic SDS, cationic DTAC, zwitterionic DDAO, and nonionic C12E8 spherical micelles in solution”, *J. Mol. Liq.* 217, 99-102(2015). DOI:10.1016/j.molliq.2015.12.062
- [2] Kawada, S.; Komori, M.; Fujimoto, K.; Yoshii, N.; Okazaki, S. “Molecular dynamics study of the formation mechanisms of ionic SDS and nonionic C12E8 micelles and n-dodecane droplets”, *Chem. Phys. Lett.* 646, 36-40(2016). DOI: 10.1016/j.cplett.2015.12.062
- [3] Wang, L.; Fujimoto, K.; Yoshii, N.; Okazaki, S. “A molecular dynamics study of the breathing and deforming modes of the spherical ionic SDS and nonionic C12E8 micelles”, *J. Chem. Phys.* 144, 034903(2016). DOI: 10.1063/1.4940031
- [4] Andoh, Y.; Muraoka, S.; Okazaki, S. “Molecular dynamics study of lipid bilayers modeling the plasma membranes of mouse hepatocytes and hepatomas”, *J. Chem. Phys.* 144, 084104(2016). DOI: 10.1063/1.4942159

- [5] Kitabata, M.; Fujimoto, K.; Yoshii, N.; Okazaki, S. “A molecular dynamics study of local pressures and interfacial tensions of SDS micelles and dodecane droplets in water”, *J. Chem. Phys.* 144, 224701(2016) DOI: 10.1063/1.4953405

Uchida, Shunsuke

Research consultant, Nuclear Safety Research Center
Japan Atomic Energy Agency, Telephone: +81 29 282 6087
2-4 Shirane, Shirakata, Tokai-mura, 319-1195 Japan Facsimile: +81 29 282 6122
e-mail: uchida.shunsuke@jaea.go.jp

- [1] S. Uchida, M. Naitoh, H. Okada, M. Pellegrini, M. Osakabe, A. Achilli and Y. Hanamoto, “An approach toward evaluation of FP behavior in NPPs under severe accident”, *Proc. 16th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-16)*, Hyatt Regency Chicago, Chicago, IL, USA, August 30-September 4, 2015.(in CD).
- [2] S. Uchida, A. Itoh, M. Naitoh, H. Okada, H. Suzuki, Y. Hanamoto, M. Osakabe, and M. Fujikawa, “Temperature dependent fission product removal efficiency due to pool scrubbing”, *Nucl. Eng. Design*, **298**, 201-207 (2016).
- [3] S. Uchida, S. Hanawa and D. H. Lister, “Advanced Water Chemistry Control Based on Parameters Determined with Plant Simulation Models”, *Power Plant Chemistry*, **17** (6), 328-339 (2015).
- [4] S. Uchida, S. Hanawa, J. Kysela and D. H. Lister, “Corrosion of structural materials and electrochemistry in high temperature water - Relationships of water chemistry, corrosion, oxide film and electrochemical corrosion potential”, *Power Plant Chemistry*, **18** (1) 6-17 (2015).
- [5] S. Uchida, H. Okada, M. Naitoh, F. Kojima, S. Koshizuka and D. H. Lister, “Improving Plant Reliability Based on Inspection and Maintenance of Local Wall Thinning due to Flow-Accelerated Corrosion”, *Proc. Int. Conf. on Flow Accelerated Corrosion, FAC2016*, May 24-27, 2016, Lille, France, EDF (2016) (in CD).**

Tsuchiya, Noriyoshi

Graduate School of Environmental Studies, Tohoku University
email: tsuchiya@mail.kankyo.tohoku.ac.jp

- [1] N. Watanabe, K. Sakurai, T. Ishibashi, Y. Ohsaki, T. Tamagawa, M. Yagi, N. Tsuchiya, “New v-type relative permeability curves for two-phase flows through subsurface fractures”, *Water Resource Research* **51**,1-18(2015).
- [2] R. Oyanagi, A. Okamoto, N. Hirano, N. Tsuchiya, “Competitive hydration and dehydration at olivine-quartz boundary revealed by hydrothermal experiments: Implications for silica metasomatism at the crust-mantle boundary”, *Earth and Planetary Science Letters*, **425**, 44-55 (2015).
- [3] T. Ishibashi, N. Watanabe, N. Hirano, A. Okamoto, N. Tsuchiya, “Beyond-laboratory-scale prediction for channeling flows through subsurface rock fractures with heterogeneous aperture distributions revealed by laboratory evaluation”, *J. Geophysical Research: Solid Earth*, **120**(1), 106-124 (2015).

- [4] S. Yamasaki, A. Takeda, T. Watanabe, K. Tagaki, S. Uchida, H. Takada, Y. Matsunami, N. Kihou, N. Tsuchiya, "Bromine and iodine in Japanese soils determined with polarizing energy dispersive X-ray fluorescence spectrometry.", *Soil Science and Plant Nutrition*, **61**, 751-760 (2015).

Adschiri, Tadafumi

Professor, Wpi- AIMR, Tohoku University

email: ajiri@tagen.tohoku.ac.jp

URL: http://www.wpi-aimr.tohoku.ac.jp/ajiri_lab/

- [1] Y.Z. Zhu, S. Takami, GY. Seong, M. Dejhosseini, M.Z. Hossain, T. Noguchi, D. Hojo, N. Aoki, T. Aida, T. Adschiri, "Green solvent for green materials: a supercritical hydrothermal method and shape-controlled synthesis of Cr-doped CeO₂ nanoparticles", *Philosophical Transactions of the Royal Society A-Mathematical Physical and Engineering Sciences*, **373**, 20150012 (2015), DOI: 10.1098/rsta.2015.0012
- [2] A. Sikora, F.F. Canova, K. Kim, H. Nakazawa, M. Umetsu, I. Kumagai, T. Adschiri, W. Hwang, W. Teizer, "Behavior of Kinesin Driven Quantum Dots Trapped in a Microtubule Loop", *ACS Nano*, **9**, 11003-11013(2015) DOI: 10.1021/acsnano.5b04348
- [3] T. Fujii, S. Kawasaki, A. Suzuki, T. Adschiri, "High-Speed Morphology Control of Boehmite Nanoparticles by Supercritical Hydrothermal Treatment with Carboxylic Acids", *Crystal Growth & Design*, **16**, 1996-2001(2016)DOI: 10.1021/acs.cgd.5b01584
- [4] N. Aoki, A. Sato, H. Sasaki, A.A. Litwinowicz, G. Seong, T. Aida, D. Hojo, S. Takami, T. Adschiri, "Kinetics study to identify reaction-controlled conditions for supercritical hydrothermal nanoparticle synthesis with flow-type reactors", *J. Supercrit. Fluid*, **110**, 161-166(2016) DOI: 10.1016/j.supflu.2015.11.015
- [5] K. Sugioka, K. Ozawa, M. Kubo, T. Tsukada, S. Takami, T. Adschiri, K. Sugimoto, N. Takenaka, Y. Saito, "Relationship between size distribution of synthesized nanoparticles and flow and thermal fields in a flow-type reactor for supercritical hydrothermal synthesis", *J. Supercrit. Fluid*, **109**, 43-50 (2016) DOI: 10.1016/j.supflu.2015.11.008

Matubayasi, Nobuyuki

Professor, Graduate School of Engineering Science, Osaka University

email: nobuyuki@cheng.es.osaka-u.ac.jp

URL: <http://www.cheng.es.osaka-u.ac.jp/matubayasi/english/index.html>

- [1] Shimizu, S.; Stenner, R.; Matubayasi, N. "Gastrophysics: Statistical thermodynamics of biomolecular denaturation and gelation from the Kirkwood-Buff theory towards the understanding of tofu", *Food Hydrocolloids*, **62**, 128-139 (2017). DOI: 10.1016/j.foodhyd.2016.07.022
- [2] Nicol, T. W. J.; Matubayasi, N.; Shimizu, S. "Origin of nonlinearity in phase solubility: solubilisation by cyclodextrin beyond stoichiometric complexation" *Phys. Chem. Chem. Phys.*, **18**, 15205-15217 (2016). DOI: 10.1039/c6cp01582d

- [3] Date, A.; Ishizuka, R.; Matubayasi, N. “Energetics of nonpolar and polar compounds in cationic, anionic, and nonionic micelles studied by all-atom molecular dynamics simulation combined with a theory of solutions”, *Phys. Chem. Chem. Phys.*, **18**, 13223-13231 (2016). DOI: 10.1039/c6cp01834c
- [4] Shintani, M.; Matubayasi, N. “Morphology study of DMPC/DHPC mixtures by solution-state ^1H , ^{31}P NMR, and NOE measurements”, *J. Mol. Liq.*, **217**, 62–69 (2016). DOI: 10.1016/j.molliq.2015.10.003
- [5] Mogami, G.; Suzuki, M.; Matubayasi, N. “Spatial-Decomposition Analysis of Energetics of Ionic Hydration”, *J. Phys. Chem. B*, **120**, 1813-1821 (2016). DOI: 10.1021/acs.jpcc.5b09481
- [6] Yamamori, Y.; Ishizuka, R.; Karino, Y.; Sakuraba, S.; Matubayasi, N. “Interaction-component analysis of the hydration and urea effects on cytochrome *c*”, *J. Chem. Phys.*, **144**, 085102 (14 pages) (2016). DOI: 10.1063/1.4941945
- [7] Ishizuka, R.; Matubayasi, N. “Self-Consistent Determination of Atomic Charges of Ionic Liquid through a Combination of Molecular Dynamics Simulation and Density Functional Theory”, *J. Chem. Theory Comput.*, **12**, 804-811 (2016). DOI: 10.1021/acs.jctc.5b00885
- [8] Stenner, R.; Shimizu, S.; Matubayasi, N. “Gelation of carrageenan: Effects of sugars and polyols”, *Food Hydrocolloids* **54**, 284-292 (2016). DOI: 10.1016/j.foodhyd.2015.10.007
- [9] Kamo, F.; Ishizuka, R.; Matubayasi, N. “Correlation analysis for heat denaturation of Trp-cage miniprotein with explicit solvent”, *Protein Sci.*, **25**, 56-66 (2016). DOI: 10.1002/pro.2754
- [10] Takahashi, H.; Matubayasi, N. “Development of a Massively Parallel QM/MM Approach Combined with a Theory of Solutions”, *Quantum Modeling of Complex Molecular Systems (Challenges and Advances in Computational Chemistry and Physics 21)*, page 153-196, edited by J.-L. Rivail, M. Ruiz-Lopez, and X. Assfeld, Springer (2015); ISBN 978-3-319-21626-3. DOI 10.1007/978-3-319-21626-3
- [11] Yoshida, K.; Matubayasi, N.; Nakahara, M.; Uosaki, Y.; “Effect of Rotation on Vibrational Spectrum of Supercritical Water: Analysis of Dependencies on Density and Hydrogen Isotopes”, *The Review of High Pressure Science and Technology*, **26**, in press (2016).

Watanabe, Yutaka

Department of Quantum Science and Energy, Graduate School of Engineering, Tohoku University

email: yutaka.watanabe@qse.tohoku.ac.jp

- [1] Fethi Hamdani, Hiroshi Abe, Benoit Ter-Ovanessian, Bernard Normand, and Yutaka Watanabe, "Effect of Chromium Content on the Oxidation Behavior of Ni-Cr Model Alloys in Superheated Steam", *Metallurgical and Materials Transactions A*, **46A** (2015), 2285-2293.
- [2] Hiroshi Abe, Seung Mo Hong, Yutaka Watanabe, "Oxidation behavior of austenitic stainless steels as fuel cladding candidate materials for SCWR in superheated steam", *Nuclear Engineering and Design*, **280** (2014), 652-660.

Kometani, Noritsugu

Associate Professor, Department of Applied Chemistry & Bioengineering, Osaka City University

email: kometani@a-chem.eng.osaka-cu.ac.jp,

URL: http://www.a-chem.eng.osaka-cu.ac.jp/kometani_group/index.html

- [1] Kometani, N.; Tanabe, M.; Su, L.; Yang, K.; Nishinari, K. “In Situ Observations of Thermoreversible Gelation and Phase Separation of Agarose and Methylcellulose Solutions under High Pressure”, *J. Phys. Chem. B*, **119**, 6878–6883 (2015). DOI: 10.1021/acs.jpcc.5b03632
- [2] Yamanashi, M.; Kometani, N.; Tsuji, K. “Preliminary experiment of X-ray diffraction imaging”, *Nucl. Instrum. Meth. B*, **355**, 272–275 (2015). DOI: 10.1016/j.nimb.2015.02.049
- [3] Kitado, Y.; Hirano, S.; Kometani, N.; Tsuji, K. “Confocal Micro XRF Monitoring of Displacement Plating Process”, *Adv. X-ray. Chem. Anal. Japan*, **46**, 269-276 (2015).
- [4] Tsuji, K.; Matsuno, T.; Takimoto, Y.; Yamanashi, M.; Kometani, N.; Sasaki, Y. C.; Hasegawa, T.; Kato, S.; Yamada, T.; Shoji, T.; Kawahara, N. “New developments of X-ray fluorescence imaging techniques in laboratory”, *Spectrochim. Acta B*, **113**, 43–53 (2015). DOI: 10.1016/j.sab.2015.09.001
- [5] Kometani, N.; Takami, R.; Nakao, K. “Advanced Treatment of Polluted Water Containing Chlorinated Organic Compounds by the Hydrothermal Oxidation Technique Using Copper Oxide Catalyst”, *Japanese J. Multiphase Flow*, **29**, 302-308 (2015). DOI: 10.3811/jjmf.29.302

Uchida, Hiroshi

Senior Research Scientist, Research and Development Center for Global Change, Japan Agency for Marine-Earth Science and Technology

email: huchida@jamstec.go.jp

- [1] Uchida, H.; Nakano, T.; Tamba, J.; Widiatmo, J.V.; Yamazawa, K.; Ozawa, S.; Kawano, T.; “Deep ocean temperature measurement with an uncertainty of 0.7 mK”, *J. Atmos. Oceanic Technol.*, **32**, pp.2199-2210 (2015). (DOI: 10.1175/JTECH-D-15-0013.1)