*Attachment 3*

# IAPWS Symposium 2017

**Wednesday, 30 August**

**9:00－9:10**

**Opening remarks, Symposium information**

## Helmholtz Awarding and Lecture

**9:10－9:40**

Dr. Pavel Gotovtsev (National Research Centre "Kurchatov Institute", Russia)

“Application of Machine Learning for Water Technologies? from Power Cycle Chemistry to Green Cities”

## Symposium Lectures

## "Water and Steam: Energy Efficiency and Environmental Sustainability"

**9:40－10:30 Session 1**

**Chair: Prof. Kenji Yasuoka (Keio University)**

Prof. Nobuyuki Matubayasi (Osaka University)

"Polymer as Energy-Saving Medium for Water Absorption: All-Atom Analysis toward Rational Design"

Dr. Ken Yoshida (Tokushima University)

"Self-Diffusion Coefficients of Sub- and Supercritical Water: Available Data, Reliable Fitting Functions, and Effects of Temperature and Density"

**10:30－10:50 Coffee break**

**10:50－11:40 Session 2**

**Chair: Prof. Nobuyuki Matubayasi (Osaka University)**

Dr. Hiroshi Uchida (Japan Agency for Marine-Earth Science and Technology)

"Long-Term Change in the Deep Ocean Resulting from Global Warming"

Prof. Kenji Yasuoka (Keio University)

"Molecular Simulation for Clathrate Hydrate"

**11:40－13:20 Lunch**

**13:20－14:35　Session 3**

**Chair: Dr. Hideo Hirano (Former CRIEPI)**

Prof. Shozo Kaneko (University of Tokyo)

“Development of High Efficiency Air-blown IGCC”

Mr. Masaki Iijima (Mitsubishi Heavy Industries, Ltd.)

“Commercialize Flue Gas $CO_2$ Capture from Power Plant”

Dr. Ayumu Morita (Hitachi, Ltd.)

"Technical Issues of Future Power Network with a Large Amount of Renewable Energy Sources"

**14:35－14:55　Coffee break**

**14:55－16:35　Session 4**

**Chair: Prof. Koichi Watanabe (Keio University)**

Mr. Nobuo Okita (Toshiba)

“Steam Turbine Cycles for Renewable Energies – Geothermal, Solar Thermal and Binary Generation –”

Dr. Hideo Hirano (Former CRIEPI)

“Current Status of Combined Cycle/HRSG Power Plant and Ultra-Supercritical Steam Power Plant, and Development of Advanced Ultra-Supercritical Steam Power Plant”

Dr. Shigeki Senoo (Mitsubishi Hitachi Power Systems, Ltd.)

“Nonequilibrium Condensation Model and Numerical Analysis for Wet Steam Turbines”

Prof. Tadashi Tanuma (Teikyo University)

“Aerodynamic Blade Designs Including Wet Steam Turbine Stages”

**16:35－16:40**

**Closing remarks**

**Polymer as Energy-Saving Medium for Water Absorption: All-Atom Analysis toward Rational Design**

**Nobuyuki Matubayasi**
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Polymer emerges as a material for selective absorption of small molecules. It plays key roles in such processes as desalination and gas separation, and the energy consumption at separation often reduces with polymer membrane compared to conventional distillation. Separation with polymer is distinct from distillation in that while the latter relies upon macroscopic phase diagrams, a rational design of the former requires insights into intermolecular interaction at atomic resolution. Atomistic analysis is thus necessary for the polymer medium, and molecular dynamics (MD) simulation is a method for meeting this necessity. In the present work, we develop a free-energy method for assessing the extent of water absorption into polymer [1]. We treat the polymer as a solvent and water as a solute, and employ a theory of solutions to accurately and efficiently compute the free energy of water dissolution [2]. It is demonstrated that all-atom treatment is predictive for the free energy irrespective of the hydrophobicity and hydrophilicity of the polymer, and the computed free energy of dissolution is discussed in connection to the structures of the polymers and their interactions with water.

**References**

[1] T. Kawakami et al., J. Chem. Phys., **137**, 234903 (2012).
[2] S. Sakuraba et al., J. Comput. Chem., **35**, 1592 (2014).

**Self-Diffusion Coefficients of Sub- and Supercritical Water: Available Data, Reliable Fitting Functions, and Effects of Temperature and Density**

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The dynamic insights into water and steam at high temperatures are of great importance to develop the high-performance power generation that is associated with efficient transformation of the kinetic energy into the mechanical. To the end the self-diffusion coefficient data is required because it represents water mass transport phenomenon. We have proposed a useful and reliable scaling law for the self-diffusion coefficients of water, that can be applied over a wide range of thermodynamic states from ambient to the supercritical [1]. The scaled expression can be used for the correlation and evaluation of the available literature data. It can be applied also for the inter- and extrapolation to the practically inaccessible extreme conditions using molecular dynamics (MD) simulation as a key guide. It has been clarified that the self-diffusion is characterized by the large temperature effect and relatively small density effect due to the attractive and directional hydrogen bonding of water [2].

**References**

[1] K. Yoshida, N. Matubayasi, Y. Uosaki and M. Nakahara, J. Chem. Eng. Data, **55**, 2815 (2010).
[2] K. Yoshida, N. Matubayasi, Y. Uosaki and M. Nakahara, J. Chem. Phys., **137**, 194506 (2012); Id. J. Chem. Phys., **138**, 134508 (2013); Id. J. Solution Chem., **43**, 1499 (2014).

## Long-term Change in the Deep Ocean Resulting from Global Warming

**Hiroshi Uchida**

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The Earth's climate system is driven by energy from the sun. Ocean and atmosphere circulations transfer this energy from the Earth's surface at low latitudes to higher latitudes. The ocean's central role in the climate system results from its great capacity to store and transport heat and freshwater to exchange these with the atmosphere. The surface water cooled around the Antarctica sinks to the bottom and forms the bottom water by spreading to all over the world ocean. To obtain an accurate picture of ocean circulation, land-to-land and surface-to-bottom global hydrographic data were gathered in the World Ocean Circulation Experiment (WOCE) in the 1990s. In the 2000s, reoccupations of the WOCE hydrographic sections have been carried out to document decadal changes of the ocean circulation. In this study, long-term changes of water properties (temperature, salinity and dissolved oxygen) and volume transport of the bottom water in the North Pacific were examined based on those high-quality hydrographic data repeatedly obtained along zonal WOCE sections at 47ºN, 30ºN and 25ºN. For depths below 4000 m, significant trends were detected for temperature (1.5±0.09 mK per decade) and dissolved oxygen (-0.99±0.12 μmol/kg per decade), although salinity trend was not significant. Half of the decrease in oxygen could be described by the isotherm heave associated with the bottom water warming. The rest of the decrease in oxygen might be casued by remineralization due to increasing residence time probably caused by slowing the deep meridional overturning circulation resulting from Global Warming.

## Molecular Simulation for Clathrate Hydrate

**Kenji Yasuoka**

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Clathrate hydrates of natural gas are suitable for industrial use such as transportation and storage. Clathrate hydrates are crystalline compounds composed of guest substances and hydrogen-bonded host water molecules. Molecular simulation is useful for studying clathrate hydrates. To clarify the thermodynamic stability of clathrate hydrate molecular dynamics simulations were applied and the free energy of clathrate hydrates were estimated [1]. Molecular vibrations of guest molecules in hydrate cages were calculated by *ab initio* molecular dynamics simulations [2]. Cage occupancy of guest molecules were also simulated by Gibbs ensemble Monte Carlo simulations [3]. Nucleation phenomena of clathrate hydrates were studied [4]. Phase equilibrium conditions were estimated by a statistical thermodynamics model [5].

**References**

[1] Y. Okano and K. Yasuoka, J. Chem. Phys. **124**, 024510(2006).; T. Miyoshi et al., J. Chem. Phys., **126**, 234506(2007).; T. Miyoshi et al., J. Phys. Chem. C, **111**, 3799(2007).; T. Miyoshi et al., Molecular Simulation, **33**, 65(2007).

[2] M. Hiratsuka et al., J. Chem. Phys., **136**, 044508(2012).; J. Chem. Phys. **137**, 144306 (2012).; Molec. Simul., **41**, 813 (2015).; Phys. Chem. Chem. Phys., **17**, 12639 (2015).

[3] P. E. Brumby et al., Fluid Phase Equilibria, **413**, 242 (2016).

[4] D. Yuhara et al., Faraday Discussions, **179**, 463 (2015).

[5] E. Sato et al., Jpn. J. Appl. Phys., **46**, 5944-5950(2007).; F. Takeuchi et al., Int. J. Thermophys., **30**, 1838(2009).

## Development of High Efficiency Air-blown IGCC

## (IGCC: Integrated coal Gasification Combined Cycle)

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Japan imports 96% of its fossil fuels from abroad. From the standpoint of energy security, Japanese Government decided the Guideline for Energy Mix 2030 aiming at 27% by natural gas and 26% by coal on power generation(kWh) basis. On the other hand Japan declared ambitious 26% reduction of $CO_2$ from 2013 result. Raising efficiency of coal fired power plant is of the first priority technical requirement. Japan has undergone development of air-blown IGCC(Integrated coal gasification Combined Cycle) technology for more than 30 years, starting from small 2 tons/day PDU(Process Development Unit) in 1982, then 200 tons/day Pilot Plant and finally 250MW IGCC Demonstration Project. The 250MW Demonstration Plant started operation in 2008 and completed successfully in 2013 after fulfilling all the targets [1]. Two commercial scale IGCCs of 540MW each are decided to be constructed as the Fukushima Restoration projects, one in Nakoso in Iwaki City, the other in Hirono, Hirono-cho both in Fukushima Prefecture. Hirono IGCC site is only 20 km away from Fukushima-Daiichi Nuclear Power Station of Tokyo Electric Power Company. Construction work already started for Nakoso IGCC Plant which will start commercial operation in mid-2020, supplying eelectricity to Tokyo Metropolitan Area serving the Tokyo Olympic Games in 2020.

[1] S. Kaneko, J.of Energy Engineering E4015018(2015), American Society of Civil Engineers.

## Commercialize Flue Gas $CO_2$ Capture from Power Plant

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Mitsubishi Heavy Industries, LTD.(MHI) started R&D since 1990 together with The Kansai Electric Power Company (KEPCO) targeting power plant flue gas $CO_2$ capture for the purpose of global warming prevention.

MHI has delivered various commercial flue gas $CO_2$ capture plants for chemicals and general use such as urea, methanol and beverages since 1999.

Power plant flue gas $CO_2$ capture is the final target for Enhanced Oil Recovery (EOR) and $CO_2$ Capture and Storage (CCS) purposes, and recently MHI delivered largest (4,776 Ton/D) coal fired power plant flue gas $CO_2$ capture plant in the world for EOR purposes in Texas USA.

How MHI carried out the R&D and increased the experiences based on commercial plants and demonstration plant are presented.

**References**

[1] Takashi Kamijo et.al. KM CDR process project update and new novel solvent development, International Conference on Greenhouse Gas Control Technologies 13 2016.
[2] Takashi Kamijo et.al. Development of the World’s Largest Post-Combustion Carbon Capture Plant for Coal-fired Power Plant MHI Technical Reports 2015.

**Technical Issues of Future Power Network with a Large Amount of Renewable Energy Sources**

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Renewable energy penetration is soaring worldwide. For instance, the added capacity in 2016 is 138.6GW, or approximately the total capacity of Canada. In Japan, in accordance to the Basic Energy Plan of the government, generation through renewable energy sources will be increased from 8.5% to 22-24% between 2015 to 2030 in order to comply with the of $CO_2$ emission reduction in COP21. As a contributer to this effort, Hitachi has provided many mega-solar systems and wind turbines, and will continue to develop advanced models. One key technology for this effort is our unique down-wind type turbine. This is a wind turbine that efficiently captures wind with the weatherclock effect by placing the turbine on the downwind side of the tower.

When installing a large amount of photovoltaics (PV) and wind turbines (WT), Japan expects to face various network issues. Generating 20% of electricity through renewable energy sources would propose two major issues. First is a shortage of tranmission capacity. Deployment of PV and WT is concentrated in areas with good weather, northern Japan, while demand would be concentrated towards the center—such as Tokyo. This would require us to enhance transmission system to increase capacity. Another issue is network instability.

Since PV and WT are unstable energy sources with power conditioning system, voltage and frequency fluctuations would occur in steady-state operation and influence of contingencies would be much greater due to lack of synchronous inertia. To solve these issues, we propose an integrated control concept, where generators, networks and consumers work together. In this presentation, system integrity protection scheme (SIPS) for a wide-area network and virtual power plant (VPP) for a local area are introduced as elements to the integrated control concept.

**Steam Turbine Cycles for Renewable Energies: Geothermal, Solar thermal and Binary Generation**

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Renewable energy systems (RES) focused on reduction of carbon dioxide have been recently considered as practical alternatives to fossil fuel power plant. In such RES, steam turbine cycles are adopted to produce stable and reliable electricity. Geothermal energy system is known as one of the most stable RES, however its resources area is limited to volcanic area or hot spring fields. Toshiba and other Japanese suppliers of turbines for geothermal systems have wide experience in various kinds of geothermal cycle over the world. We have faced issues such as erosion/corrosion by the wet steam mixed with non-condensable gases and impurities and measuring method of wetness. Some items are resolved but some still partly remain.

Another renewable steam cycle is a solar thermal system well known as CSP. It is also limited to sunny places and it supplies unstable power with low temperature and moist exhaust steam. Nevertheless, the solar system combined with biomass boiler and binary generation can supply more stable power even at lower heat area like in Japan. Binary turbine and its combination with flash steam turbine would also contribute to use geothermal resources effectively and widely to lower temperature and more gas mixture in the steam.

We would be able to plan and offer practical RES with more efficient and economical steam turbine cycles based on our experiences and by the expectation to IAPWS of solving issues on water, steam and aqueous solutions as working fluid and heat transfer fluid.

**Current Status of Combined Cycle/HRSG Power Plant and Ultra-Supercritical Steam Power Plant, and Development of Advanced Ultra-Supercritical Steam Power Plant**

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As for the combined cycle/HRSG power plant, Higashi-Niigata thermal power plant began commercial operation as the first Japanese combined cycle power plant in December, 1984. For about 33 years after 1984, the 23 combined cycle/HRSG power plants including 130 units have been installed until July 31, 2017. All combined cycle/HRSG power plants use the LNG for fuel. On the other hand, as for the Ultra-Super Critical (USC) power plant, Kawagoe thermal power plant started commercial operation as the first Japanese USC power plant in June, 1989. For about 28 years after 1989, the 17 USC power plants including 27 units have been installed until July 31, 2017. Almost all USC power plants use the coal for fuel.

Although some problems are left behind on both the combined cycle/HRSG power plant and USC power plant, the thermal efficiency of combined cycle/HRSG power plants were improved from 48.6% LHV to 61% LHV, and the thermal efficiency of USC power plants were improved from 43% LHV to 45% LHV, respectively. The combined cycle/HRSG power plant and USC power plant have been positioned as the main source of power generation in Japan. In recent years, from a viewpoint of $CO_2$ reduction of global warming prevention, improvement in the further efficiency is required, and the development and utilization of the 1700ºC class combined cycle/HRSG power plant and Advanced-USC power plant are progressing.

**References** : [1] S. Nakamura et. al. Technical Development and Future Prospect of A-USC, MHI Technical Report Vol.48, No.3, 2011. (In Japanese)

**Nonequilibrium condensation model and numerical analysis for wet steam turbines**

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In most conventional power plants the steam turbines are supplied with superheated steam but, during the course of its expansion, the condition of the steam enters the two-phase region and the last few low-pressure stages operate in the wet regime. The main practical consequences of operating in the wet regime are blade erosion and corrosion damage, and deterioration in thermal efficiency due to a variety of two-phase effects collectively known as wetness losses. The adverse impact of condensation on efficiency has been appreciated from the very early days of steam turbines and considerable progress has been made in many aspects of condensing-flow research. Three dimensional, nonequilibrium calculations are now possible for multistage turbines, even fundamental uncertainties remain regarding nucleation and droplet growth models, and numerical methods are still unable to predict the broad droplet size distributions observed in real turbines. The derivation of theories for nucleation and droplet growth to model droplet size spectra in nonequilibrium condensating steam flow will be presented together with both numerical and experimantal results in the latest international collaboration project [1].

**References**

[1] Senoo, S., and White, A.J., Chap.9: Analysis and Design of Wet Steam Stages, Advances in Steam Turbines for Modern Power Plants, Elsevier, pp.165-218, (2016)

# Aerodynamic Blade Designs Including Wet Steam Turbine Stages

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The power-generation percentage by steam turbines in all power stations including renewable energy power stations was 60% in 2012, and estimated to become 47% in 2040 [1]. Almost all turbine stages in nuclear, geothermal and concentrated solar power stations operate in wet steam conditions. Even in steam turbines for modern ultra-supercritical thermal power stations, last a few low-pressure turbine stages operate in wet steam conditions. These data show that understanding of accurate properties of wet steam flows and condensation water flows should be critical for design of blades in steam turbine stages [2]. Velocities of steam flows in steam turbine stages become high when the steam goes through throats of the flow paths and the velocities sometimes go over the sonic speed in last a few low-pressure long blade flow paths. In these conditions, non-equilibrium condensations can take place in blade flow paths and these phenomena lead to changes of pressures, velocities and flow angles of inlet and outlet of stationary and rotating blades. Aerodynamic blade designs including these wet steam turbine stages with these non-equilibrium wetness effects will be presented.

**References**

[1] T. Tanuma, Chapter 1: Introduction to steam turbines for power plants, Advances in Steam Turbines for Modern Power Plants, Elsevier, pp.3-9, (2016)

[2] T. Tanuma, Chapter 6: Design and analysis for aerodynamic efficiency enhancement of steam turbines, Advances in Steam Turbines for Modern Power Plants, Elsevier, pp.109-126, (2016)