Energy Outlook

International Institute for Carbon-Neutral Energy Research

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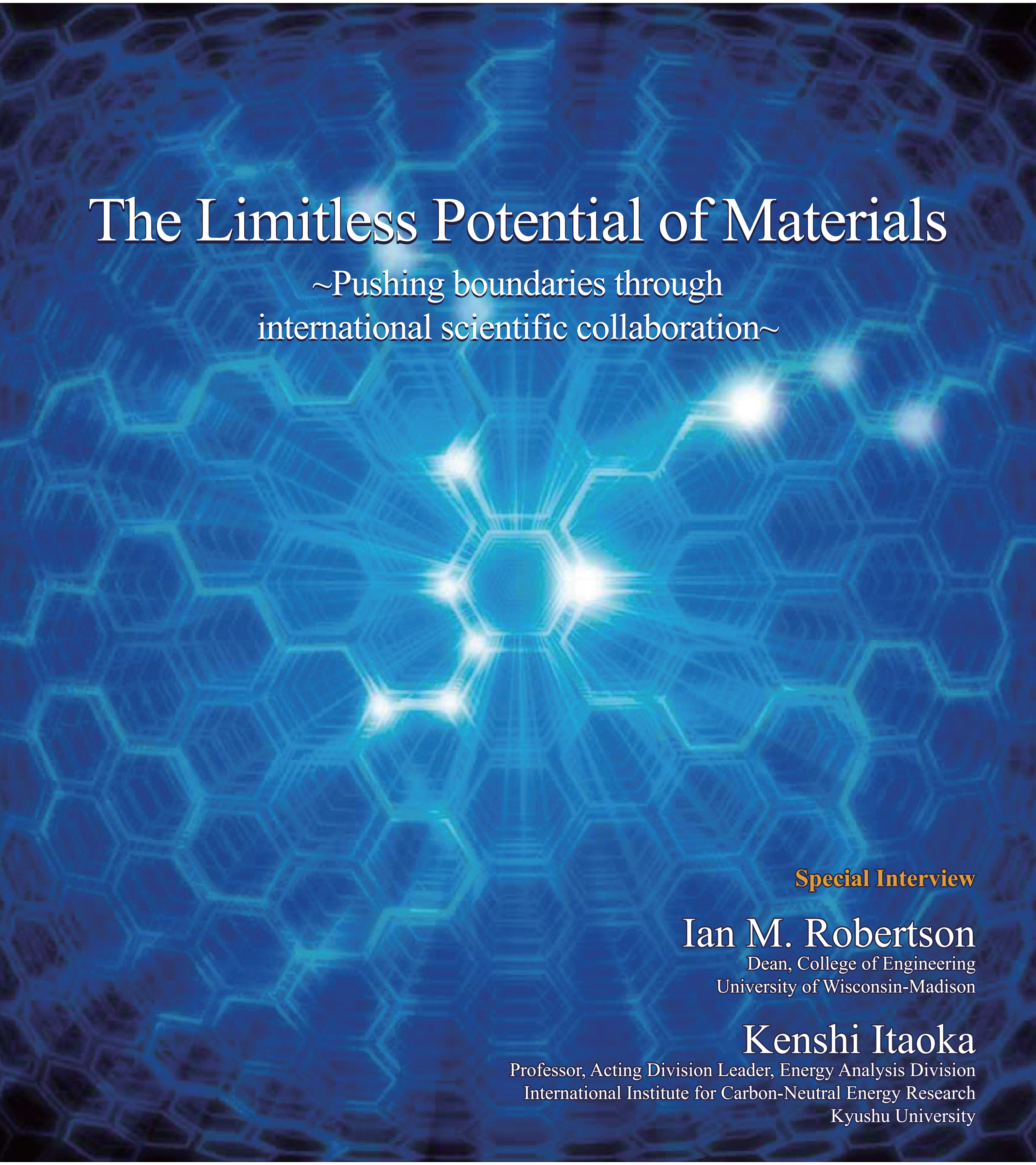

The Limitless Potential of Materials

~Pushing boundaries through international scientific collaboration~

Special Interview

Ian M. Robertson
Dean, College of Engineering
University of Wisconsin-Madison

Kenshi Itaoka
Professor, Acting Division Leader, Energy Analysis Division
International Institute for Carbon-Neutral Energy Research
Kyushu University

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Special Interview

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The Limitless Potential of Materials

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Materials science plays a key role in research efforts to increase efficiency of energy conversion and lower carbon intensity. Bringing together materials science and computational science has the potential to answer further key questions and enhance predictive methods. Integration of experimental, data, and computational tools, and collaborative efforts in data sharing can boost research innovation, leading to new applications and cost reductions on the path towards a carbon-neutral society. In this special interview, Professor Kenshi Itaoka discusses the limitless potential of materials science in all its various aspects with Dean Ian Robertson.

Ian M. Robertson

Dean, College of Engineering, University of Wisconsin-Madison

In March 2013, Dr. Ian Robertson became the ninth dean of the University of Wisconsin-Madison College of Engineering. From 2011-13, he was the Director of the Division of Materials Research for the National Science Foundation (NSF). From 2003-2009, he served as Department Head for the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. He has been a member of the materials science faculty since 1983. Robertson has received numerous teaching and research awards, including DOE awards for outstanding scientific accomplishment in metallurgy and ceramics (DOE Basic Energy Sciences, 1982), and for contributions to our understanding of mechanisms of hydrogen embrittlement (DOE EE Fuel Cell Program, 2011). Robertson is the 2014 recipient of the ASM Edward DeMille Campbell Memorial Lectureship. He received his Bachelor's in Applied Physics from Strathclyde University in Glasgow, Scotland in 1978, and his Doctor of Metallurgy from the University of Oxford in Oxford, England in 1982.

Materials science as an engine for research on energy efficiency

Kenshi Itaoka: We can follow two approaches in order to reduce greenhouse gas (GHG) emissions significantly in the future: 1) we can increase the efficiency of energy conversion or use, and 2) we can lower the carbon intensity of energy. These are the two approaches that are receiving the most attention from the research community. So can you tell me how materials science can enhance this research and what specific areas need to be prioritized?

Ian Robertson: The question you pose is very broad in scope. I think that materials science has a significant role to play in these areas. For example, if you seek to increase the operating temperature and efficiency of power conversion systems, new materials with orders of magnitude enhancements of existing properties will be required, especially if you want them to last for a long period of time in an intense operating environment. In terms of transportation, the light-weighting of vehicles is another challenge. If we can create materials that achieve weight reductions, then fuel efficiency will improve in any type of vehicle, whether it be a combustion engine, fuel cell, or electric vehicle. Although weight can only be reduced by so much before safety becomes a concern, any reductions will be significant in terms of energy usage.

Itaoka: The light-weighting of vehicles is an old topic, but it is one where there is still room for improvement and development, especially in the areas of carbon composite, plastic, and aluminum materials.

Robertson: I agree that there are opportunities in composites, polymeric systems, aluminum, and magnesium alloys. Another challenge is to make thinner plate steel with the same strength properties as the steels used today. Although light-weighting is considered to be an old research area, it is still very relevant. We still have a long way to go to improve efficiency and improve the materials we use, particularly in battery and fuel cell vehicles. In terms of fuel cell vehicles, it will also be important to consider hydrogen supply and what kind of catalysts may improve the efficiency of the conversion process. I see the cheap production of hydrogen from renewables in sufficient quantities to power a hydrogen-based economy as a major challenge. There is a major role for materials science to play in improving catalysts for hydrogen production. In terms of the vehicles themselves, it is important to consider how to recapture some of the wasted energy so it can be reused. Any way you could generate extra energy on board is important and materials has a role to play, for example, in film-type photovoltaics to create extra energy-generating capability. In the case of Japan, if there is going to be a shift to hydrogen and hydrogen-powered vehicles, another major challenge will be materials compatibility with hydrogen. The effects of hydrogen on the degradation of metals is well known, but we do not know how to predict when failure will occur. It is also going to be important to understand the hydrogen compatibility of other materials that will be used in a hydrogen-fueled vehicle.

Itaoka: Not many people appreciate the importance of compatibility. I agree that compatibility is a major topic if we are to make a hydrogen-powered world safer.

Robertson: Another challenge for materials science related to hydrogen-fueled vehicles is to make a lightweight onboard regeneration system, which would be an alternative to using a high pressure gas tank. However, a complex metal hydride that has the necessary thermodynamic and kinetic properties to operate in a vehicle has yet to be found.

Itaoka: Some people are skeptical about moving away from high-pressure storage, but as research progresses, this is something that may become feasible.

Integrating materials science with computational science

Robertson: The challenge of identifying suitable onboard lightweight hydrogen storage materials is an example of how computational science could be used to accelerate the discovery of candidate systems. For example, computational methods could identify the most promising compositions from the many thousand possibilities. This would reduce the number of compositions that had to be synthesized, processed, and tested, and it would make the challenge more tractable. I think computational materials science in conjunction with an experimental program has tremendous potential to identify a solution. Ideally, our computational tools should be able to take into account the environment in which the system will operate and, of course, we must have the capabilities to synthesize the identified system.

Itaoka: Do you think we can calculate how long materials last without major experimentation? Experiments to estimate materials durability are very difficult. Could computational science help in that regard?

Robertson: Despite the incredible progress that has been made in our computational toolkit in the last decade, being able to scale from first principle to continuum level calculations remains a challenge, especially if we are to ask about materials performance in an environment relevant to an application. This is an area in which significant improvements are needed. Experimentation will still be essential to test the predictions of simulations and models, as well as to discover new knowledge germane to the problem being investigated. The key aspect is to have them work synergistically so that they are aiding each other and guiding future directions. This coupling is one of the key aspects of the Materials Genome Initiative (MGI) .

Itaoka: Computational science could also make a contribution to the work being done at I^{2}CNER, because our current activities rely mainly on experiments. How advanced are efforts in the United States to bring together materials and computational science?

Kenshi Itaoka

Professor, Acting Division Leader, Energy Analysis Division, International Institute for Carbon-Neutral Energy Research (I^{2}CNER), Kyushu University

After graduating with a Bachelor's degree from the Department of Aesthetics and Art history, Faculty of Fine Arts, Tokyo University of the Arts in 1984, Dr. Itaoka completed the Master's program at the Department of Industrial Design, Faculty of Engineering, Chiba University in 1986. Subsequently, he completed the Master's program at the Department of Urban and Regional Planning, Faculty of Natural Resource Development and Planning, University of Wisconsin-Madison in 1992. In 2011, he received his Doctoral degree from the School of Engineering, the University of Tokyo. After working at Fujitsu General Limited and the Mizuho Information & Research Institute Inc., he joined the International Institute for Carbon-Neutral Energy Research (I^{2}CNER), Kyushu University in 2013. He accepted his current position in I^{2}CNER in November 2013.

Robertson: I agree, incorporating computational sciences into the experimental effort of I^{2}CNER is an excellent opportunity that could provide unique benefits. There are many excellent examples in which computational and experimental programs operate cooperatively and synergistically in the US. However, there is still much progress to be made, and this is one goal of the MGI effort. Unprecedented levels of advancement, cooperation, and communication within the scientific community, which are challenges in themselves, will be required to develop the next generation of algorithms which will span the appropriate spatial and temporal scales. I see this integration of computational and experimental tools as a unique opportunity for I^{2}CNER to lead the way and distinguish its efforts from those of other institutions.

Itaoka: We would need to make a focused effort to bring in computational scientists.

Robertson: Yes, and I think you would need to find computational scientists who are interested in applying their skill sets to I^{2}CNER-related problems. You would need to integrate them throughout the entire I^{2}CNER program and encourage them to interact with experimentalists and vice versa.

Itaoka: I think that the key is to make sure that people are connected, and that adequate facilities and equipment are available.

MGI is a U.S. government multi-stakeholder initiative to develop an infrastructure to accelerate and sustain domestic materials discovery and deployment in the United States. https://www.whitehouse.gov/mgi

Importance of data sharing to enhance research innovation

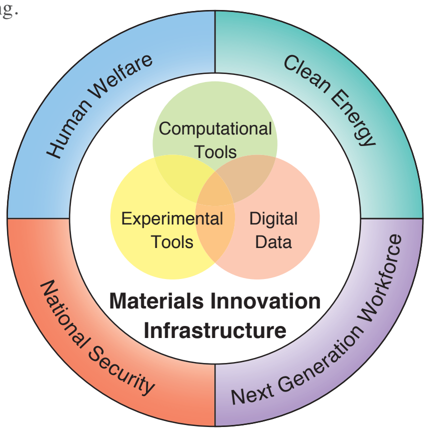
Robertson: Another issue we need to consider relates to data. A great deal of data relevant to establishing a hydrogen-driven economy exists, both at I^{2}CNER and globally, and if we could start sharing this data, and learning how to interrogate and visualize it, I think there are opportunities for new discoveries. Some industries have been much better at sharing data than academia. I^{2}CNER has an opportunity to become a leader in Japan by making data available broadly and thereby demonstrating leadership in research innovation.

Itaoka: At the moment, there are only bilateral agreements on sharing research datasets. It would certainly be an innovative approach to make data more widely available. Do you envisage any issues related to intellectual property arising from using such an approach?

Robertson: Yes, the intellectual property issues will need to be resolved. However, there are ways the datasets could be handled to ensure that the data is not used by others before it has been published. An initial opportunity for I^{2}CNER is for the data generated within it to be shared internally with everyone. One challenge will lie in building a system that makes this possible, including getting the scientists to record their data in an appropriate format. There are similar efforts in the US to make this possible.

Materials Innovation Infrastructure

Robertson: The key concept behind the MGI effort is the Materials Innovation Infrastructure. This has three components: 1) computational tools, 2) digital data, and 3) experimental tools (including synthesis, processing, and characterization of properties). Although there are opportunities for advances in each area, the full capability and potential is realized in the regions of intersection, especially when all three components are included. The Materials Innovation Infrastructure applies not just to materials science, but to all areas of science and engineering.



The Materials Innovation Infrastructure
Source: Materials Genome Initiative Strategic Plan, Materials Genome Initiative, National Science and Technology Council Committee on Technology, Subcommittee on the Materials Genome Initiative, December 2014.

Working with developing countries to reduce GHG emissions

Itaoka: Although China and the United States are the top emitters of GHG, the proportion emitted by developing countries continues to rise. New materials may help in reducing these countries' emissions, and improve quality of life and economic activities for their people. However, financial constraints generally mean that cheap but energy inefficient materials and equipment are used in developing countries. How can materials science help to overcome the various challenges that developing countries face?

Robertson: Education is of greatest importance. We need to show people how methods for producing energy can be applied and how technologies can be effectively utilized. We also need to be prepared to share technologies and make them available to developing countries at an affordable cost. We are still in the process of educating our own societies to be more energy efficient or use less power. We can help developing countries by passing on our knowledge and educational tools. Part of our challenge across the world is changing how the consumer looks at the availability of power.

Itaoka: As you pointed out, education and affordable cost are important factors. Even in developed countries, prohibitive costs can lead to systems not being deployed. Therefore, the challenge we face is how to develop advanced materials with enhanced function at reduced cost.

Robertson: I agree. Currently, from the discovery of a material in a laboratory to its deployment and application, the timescale in many industries is on the order of 20 years. The goals of and idea behind the MGI is to reduce this timescale considerably, and to reduce the cost at each stage in the materials development continuum. This continuum extends from the discovery phase, through the development, property optimization, systems design and integration, certification, manufacturing, and deployment phases. The latter phase should include materials sustainability and recovery, as these are going to become increasingly important areas as we exhaust the supply of natural materials. If all phases in the development continuum can run concurrently rather than linearly, there are opportunities for significant reductions in the time and cost of a new material appearing in a product.

International collaboration to advance materials science

Itaoka: How do you think I^{2}CNER can leverage its international networks on materials to advance its energy mission?

Robertson: I think that I^{2}CNER has made remarkable progress in building an international network in the areas of materials, carbon capture / storage, and fuel cells. Many international researchers and institutions are now seeking to interact with I^{2}CNER, which speaks very highly of the recognition and reputation you have built in your work on the carbon-neutral society. If you can now become a leader in data- and computational-enabled science, and show how this can be done and what can be achieved with it, the standing of I^{2}CNER as a leading scientific institution will be enhanced. The Energy Analysis Division's approach to creating roadmaps and building research into the roadmaps is very impressive, and has a big impact on the direction of I^{2}CNER. There are not many international examples where such an approach has been employed and it is an important development in order to break down research barriers.

Itaoka: Many institutes are working on similar roadmaps, but our advantage lies in the fact that we are directly connected to basic science research.

Robertson: Yes, I think that what I^{2}CNER is doing in seeking to identify the roadblocks to the accomplishment of a future hydrogen-based carbon-neutral society is a very important development. The I^{2}CNER strategy of using the roadmap as a way of guiding the research is highly innovative. While reputation is undoubtedly important, efforts now need to be made to publicize the achievements of I^{2}CNER to a wider audience and enhance awareness about the progress that is being made.

Special Interview
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Research Highlights

1 Changes in Pore Geometry and Relative Permeability caused by Carbonate Precipitation in Porous Media

Fei Jiang and Takeshi Tsuji
Physical Review E
DOI: 10.1103/PhysRevE.90.053306

The mineralization mechanism of CO_2 geological storage alters the pore structure over time, and leads to a corresponding change of permeability with time. In this study, we investigate numerically the influence of carbonate precipitation on relative permeability. The fluid velocity field within the pore spaces was calculated using the Lattice Boltzmann Method, while reactive transport with calcite deposition was modeled using an advection-reaction formulation solved by the finite volume method. We proposed new pore clogging models by transforming fluid nodes to solid nodes based on their precipitated mass level. Our model accurately simulates the mineralization process observed in the laboratory experiment. Precipitation-induced evolution of pore structure significantly influenced the absolute permeability. The relative permeability was much more heavily influenced by pore reduction in the CO_2 phase than in the water phase. This result is expected to greatly contribute to the clarification of the behavior of stored CO_2, which is one of the themes of the I^{2}CNER CO_2 Storage Division's roadmap.

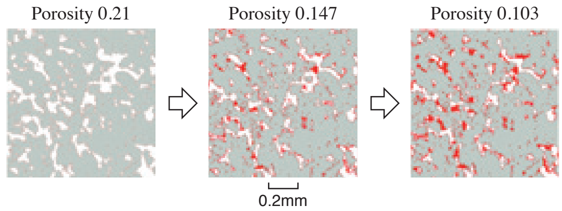

Fig. 1: The precipitation patterns of Berea sandstone at intersections perpendicular to the flow direction calculated using the new clogging model (light gray is the original grain and dark red is the precipitated regions).

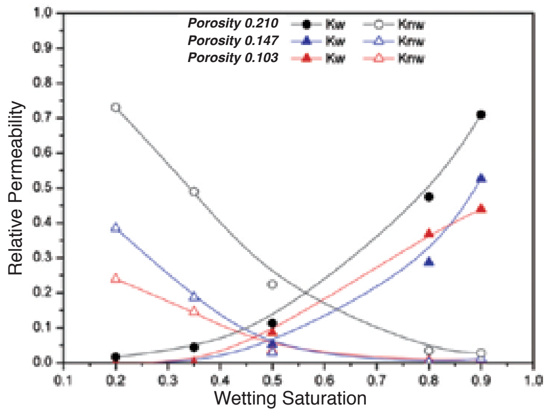

Fig. 2: Evolution of relative permeability as the porosity is altered by the clogging model (0.210–0.103). *Knw* and *Kw* represent the relative permeability of non-wetting phase (CO_2) and wetting phase (water) respectively.

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2 Non-isothermal bubble rise: non-monotonic dependence of surface tension on temperature

Manoj Tripathi, Kirti C. Sahu, George Karapetsas, Khellil Sefiane, and Omar K. Matar
Journal of Fluid Mechanics
DOI: 10.1017/jfm.2014.659

Self-rewetting fluids are working liquids with a demonstrated great potential for enhancing heat transfer. These are mixtures which have a unique property of exhibiting minimum surface tension dependence on temperature. The paper makes a fundamental contribution and provides a new insight into understanding the behavior of vapor bubbles of these self-rewetting fluids, subject to a temperature gradient. Thermal management contributes in a significant way to worldwide carbon emmisions and energy use. The ability to miniaturize thermal devices by using novel working fluids will certainly help in designing more efficient thermal cooling technologies. Creating miniturized cooling technolgies will require an understanding of the fundamentals, such as the ones revealed in this paper. Miniturization and intensification lead to lighter cooling devices in cars, airplanes,. etc. This will dramatically reduce our global energy consumption.

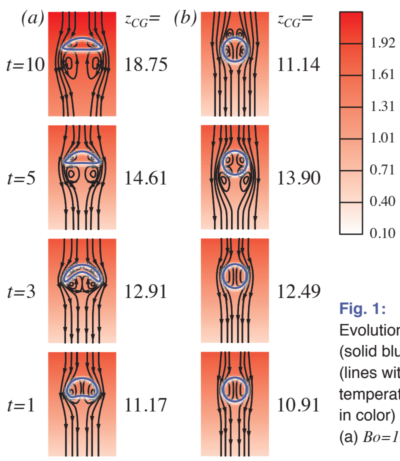


Fig. 1: Evolution of bubble shape (solid blue line), streamlines (lines with arrows), and temperature contours (shown in color) with time for (a) $Bo=10$ and (b) $Bo=10^{-2}$.

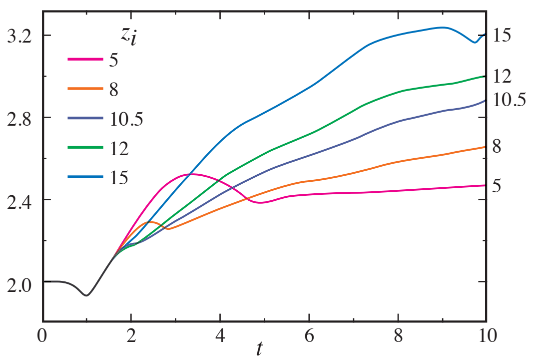


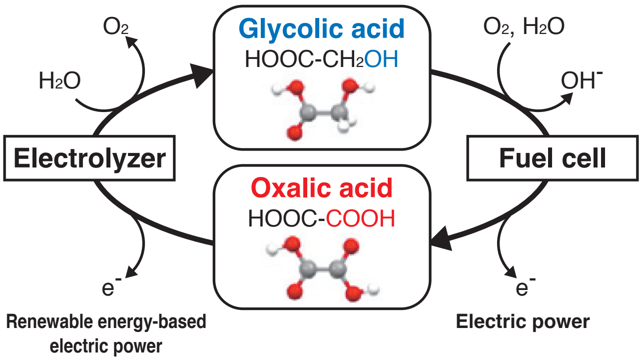
Fig. 2: The effects of the initial location of the bubble on the elongation of the bubble.

3 CO_2-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple

Ryota Watanabe, Miho Yamauchi, Masaaki Sadakiyo, Ryu Abe, and Tatsuya Takeguchi

Energy & Environmental Science
DOI: 10.1039/C5EE00192G

In view of the supply stability issues related with renewable energy, the establishment of an efficient electric power distribution methodology is the key to realizing a sustainable society that is driven by renewable energy-based electricity. Here, we demonstrate a novel electric power circulation method that does not emit CO_2 and which uses the glycolic acid (GC)/oxalic acid (OX) redox couple. Direct electric power storage into GC ensured considerable high energy density storage (8700 MJ/m^3) through the OX reduction with significantly high selectivity (>98%) using a TiO_2 catalyst under mild conditions (-0.5--0.7 V vs. the RHE, 50 ℃). We also succeeded in generating power without CO_2 emissions using the electrooxidation of GC coupled with an alkaline fuel cell. This achievement is already beyond the mid- and long-term milestones (Fuel regeneration by electrorecusion:1% (~2025) and energy circulation without CO_2 emission (~2050)) in the I^{2}CNER Catalytic Materials Transformations Division Roadmap.



A schematic diagram of CO_2-free, electric energy circulation using the GC/OX redox couple as an energy carrier.

4 Impact of Interfacial Tension on Residual CO_2 Clusters in Porous Sandstone

Fei Jiang and Takeshi Tsuji

Water Resources Research
DOI: 10.1002/2014WR016070

We develop a numerical simulation method to calculate the characteristics of CO_2 residual clusters to quantify capillary trapping mechanisms in real sandstone. A digital-rock-pore (geometry) model reconstructed from micro-CT-scanned images of Berea sandstone is filtered and segmented into a binary file. Based on this digital rock model, the CO_2 residual-cluster distribution is generated following simulation of the drainage and imbibition processes. The characteristics of CO_2 clusters in terms of size distribution, major length, interfacial area, and sphericity are investigated under conditions of different interfacial tension (IFT). It is found that high IFT increases the residual saturation and leads to a large size distribution of residual clusters. Low IFT results in a larger interfacial area, which is beneficial for dissolution and reaction processes. Analysis of the force balance acting on the residual clusters demonstrates that trapping stability is higher in the high IFT case, and the IFT should be an additional controlling factor for the trapping. Using this method, we can obtain residual-cluster distributions under different conditions for optimizing the storage capacity of carbon-storage projects.

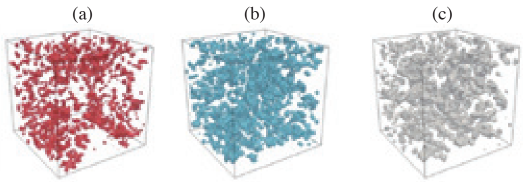


Fig. 1: Residual CO_2 clusters distributions in 3D reconstructed Berea sandstone for three cases with different IFT conditions (red: low IFT, blue: mid IFT, white: high IFT). Each cluster is isolated and trapped. Low IFT results in many small spheroid blobs, whereas high IFT leads to a distribution of large, irregular, branched clusters.

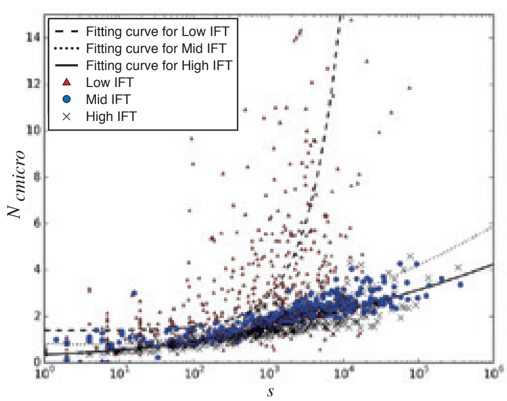


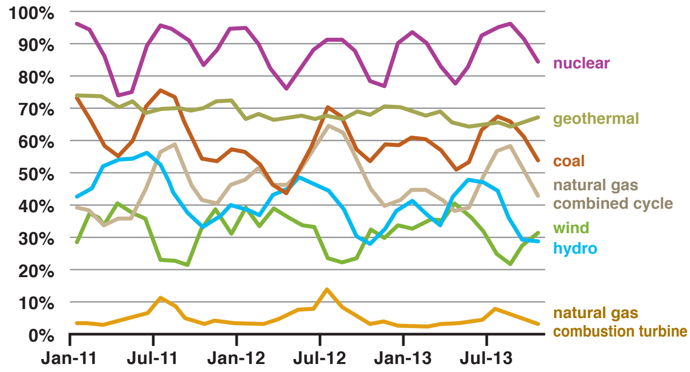
Fig. 2: The relationship between the cluster size and the calculated stability factor N_{cmicro} for the three cases with different IFTs. Trapping stability is higher in the high interfacial tension case, and N_{cmicro} increases with the volume size, larger volume cluster is unstable and should be easier to remobilize.

5 The dynamics of electricity grid operation with increasing renewables and the path toward maximum renewable deployment

Xuping Li, Mark Paster, and James Stubbins

Renewable and Sustainable Energy Reviews 47(2015)1007-1015
DOI: 10.1016/j.rser.2015.03.039

This study analyzes the dynamics and impact of renewables on the grid and identifies the bottleneck problems and solutions related to renewable integration. Variability issues that concern many are not unique to variable renewables - grid operators have been dealing with demand variability for over a century. With a sufficiently accurate forecast for variable renewables, the grid operators can balance demand and supply on a real-time basis. Base load generators operate nearly constantly for days or longer and supply a larger share of the electricity than is proportional to their capacity. This will be a limiting factor for high level variable renewables. The capability to follow electricity load should be a key performance measure of non-renewable plants to achieve high level variable renewables. Specific policy instruments are recommended to incentivize more flexible plants and ensure smooth integration of variable renewables.



Monthly capacity factors for selected fuels and technologies

6 A methodology for velocity field measurement in multiphase high-pressure flow of CO_2 and water in micromodels

Farzan Kazemifar, Gianluca Blois,
Dimitrios C. Kyritsis, and Kenneth T. Christensen

Water Resources Research
DOI: 10.1002/2014WR016787

Storage of CO_2 in deep saline aquifers (porous structures saturated with brine) has emerged as a viable solution for reducing greenhouse gas emissions while the adoption rate of renewable energy sources increases. Safe storage and trapping efficacy of injected CO_2 in these geological formations, two important goals of I^{2}CNER's CO_2 Storage Division, depends, among other factors, on the flow field during and after injection. This paper presents a novel methodology combining fluorescence microscopy and microscopic particle image velocimetry to capture instantaneous, temporally and spatially resolved velocity fields in the high-pressure, multi-phase flow of CO_2 and water through a porous micromodel. This approach provides a step-change in capability for investigating multi-phase flow physics at the pore-scale at reservoir-relevant conditions (80+ bar, 30+°C).

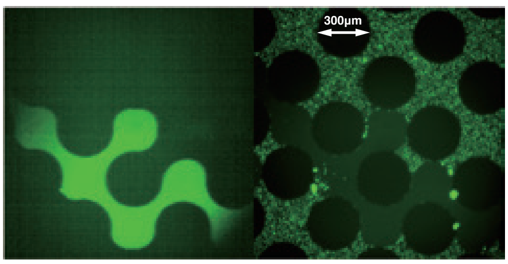


Fig. 1: (left) Dyed CO_2 image from camera 1. (right) Tracer particle image from camera 2

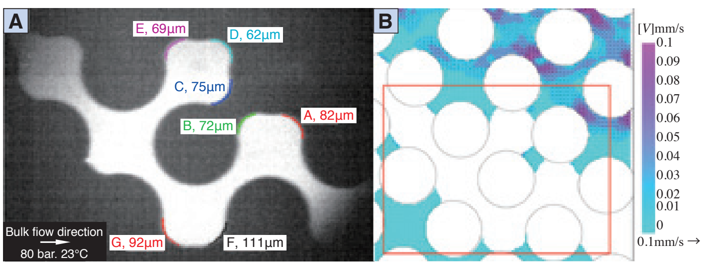


Fig. 2: (A) CO_2 fluorescent image with radius of curvature in the image plane demarcated. (B) Water velocity vector field at the same instant (the red rectangle demarcates the corresponding area in Fig. 2(A)