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G-COE PROGRAM KYUSHU UNIVERSITY

NOVEL CARBON RESOURCE SCIENCES

NEWSLETTER

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M E S S A G E

Professor of Tokyo University of Science
(Former Director-General for Regional Economic and Industrial Policy in METI)

Osamu Tsukamoto



A new path of the carbon resource industry in the 21st century—Hope for the G-COE program of NCRS—

A research and education and human resources development program in the G-COE program of “Novel Carbon Resource Sciences” (NCRS) based in Kyushu University was launched in FY2008. Recently, it has started bringing positive outcomes. The center has been engaged in a wide variety of activities whose scope is expanding more and more: the education curriculum which focuses on advanced use of coal resources; the innovative research and development including that for technologies of zero-emission coal-fired power generation and coal gasification; and the human resource development programs and international exchange of students and researchers. I would like to express my deepest respect for those who have made tireless efforts to the program. It is a great pleasure for me to see meaningful outcomes, as I took charge of forming an industrial technology policy in the Ministry of Economy, Trade and Industry, helping establish the G-COE program from the sidelines at the time of its foundation. The Industrial Structure Council pointed out the need for developing innovative technology for global environment and discussed the variety of technology development roadmaps. However, there was a dichotomy on the issue of coal resources. Some insisted on reducing coal utilization drastically because of the adverse impact on global environment, whereas others urged the importance of advanced use of coal resources. Considering the energy situation in developing countries with ongoing economic growth and the energy supply-demand structure in which even industrialized nations heavily depend on coal resources, it is a significant policy challenge how we achieve advanced use of coal resources in an environmentally-balanced manner.

Since there was a growing need for an international base which would address global environmental problems, the G-COE of NCRS was formed as a result of dedicated efforts by people concerned. The educational curriculum was completed step by step with the support of many technical experts and researchers from private sectors, under the strong leadership of Kyushu University's faculty members. I believe the start of the G-COE of NCRS led the coal industry that had helped Japan's modernization since the Meiji era, into a new path in the 21st century.

In recent years, Japan's industrial technology has been lagging significantly behind other developed countries in terms of competitiveness. “Why can't we compete in the market, even though Japan has the leading-edge technology?” “What can create a job and make a profit in Japan in the future?”. The government's new growth strategy suggests how we build a new industrial structure and an innovative strategy to help drive Japanese economy despite its population decline, which includes overseas operations of advanced energy system. We need to look up “Cloud above the Hill¹⁾ for the 21st century; aiming for a world innovation center in concert with Asia's economic growth in order to actively contribute to solutions of global environmental issues. The G-COE program of NCRS in Kyushu University was established to meet the demands of the times. I wish the G-COE program continued success and prosperity.

“It is the crucial time, keep going.” “Dream comes true, pursue the dream.”

¹⁾ Ryotaro Shiba, a famous Japanese novelist, described symbolically the ideal of nation-building which Japanese elites pursued about one hundred years ago as “Cloud above the Hill”.

Summary of G-COE Program "NOVEL CARBON RESOURCE SCIENCES"

The Global COE program of Novel Carbon Resource Sciences (NCRS) arose from a partnership between Kyushu University and Fukuoka Women's University in FY 2008. Faculty members of 8 departments in the two universities are investigating a new field of science that concentrates on the efficient use of carbon resources and global environmental protection. The education of young researchers is performed from a global perspective through advanced research. Carbon resources such as oil and coal are vital to human life, not only as energy resources, but also as chemical raw materials. Today people need to approach to the issues associated with rapid economic development, such as depletion of resources, environmental pollution and global warming. Still, carbon resources are indispensable as energy resources or chemical raw materials. Above all, coal can be found in many parts of the world with large reserves, whereas the improper use of coal can cause air pollution and large volumes of CO₂ emissions. How can we produce energy in an effective and environmentally-friendly manner, with a well-balanced approach that allows us to maintain comfortable lives? In order to address this challenge, it is essential to use carbon resources "wisely", considering a best mix with other energy.

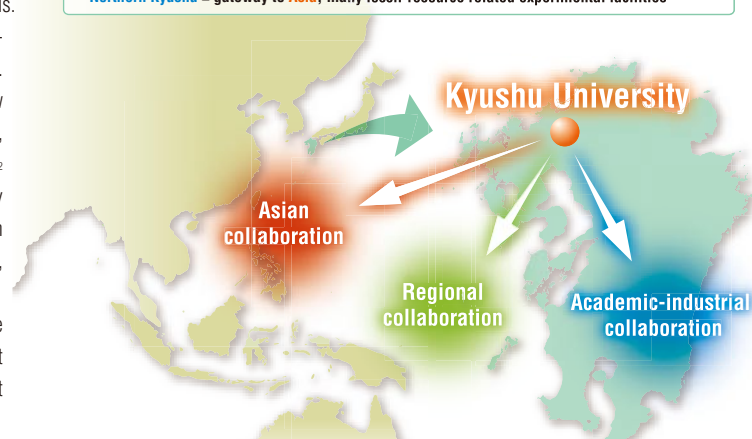
As the world is exploring various countermeasures, this COE is striving to solve the problem with the objective of creating environmentally-friendly society for the next generation. We are promoting the development of technology for the maximum efficient use of carbon resources and materials derived from carbon resources to realize a low-energy society, and encouraging the education of young researchers who will be able to help build a future strategy for overcoming practical problems through advanced research.

Two years after its foundation, our COE underwent an interim assessment in July 2010. The COE, in which more than half of students are from overseas, has been implement-

ing distinctive curriculums including the advanced research on resources, environment and energy, short-term and long-term internships, fieldworks, and the NCRS forums with the cooperation of Asian countries, urging human resource development.

Group Leader Hideo Nagashima

Kyushu University = rich history of leading coal research, future plans for an "Energy campus"
Northern Kyushu = gateway to Asia, many fossil-resource related experimental facilities



NOVEL CARBON RESOURCE SCIENCES

20th century

More indiscriminate consumption of fossil resources



21st century

More sustainable utilization of fossil resources

■ Cooperation with local community and Asian countries

The center takes full advantage of Kyushu University's location in Northern Kyushu, a gateway to Asia. We will be actively engaging in bidirectional exchanges of research and education among universities, institutes in China, Korea, Indonesia, India, Australia and Thailand collaborating internationally on education with Fukuoka

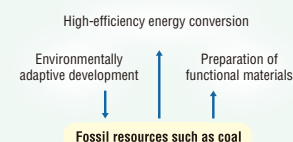
Women's University. Also, we will be sharing intelligence with people in region through public lecture and partly promoting nationwide, international joint research between industry and academia.

■ Development and integration of two research fields

This COE pursues: in carbon resource utilization field, smart use of carbon resources such as coal that is extremely effective energy use and energy-saving material, device and system derives carbon resources. At the same time, to figure out environmental change and find a solution mutually by economic, science and engineering in carbon resource environment field. This COE aims at establishing new integrated research field 'Novel Carbon Research Sciences'.

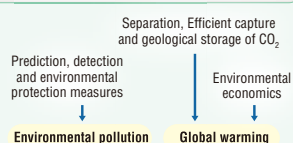
Carbon Resource Utilization

- a) Basic research in the environmentally benign development of fossil resources such as coal and high-efficiency energy conversion technologies (Clean Coal Technology)
- b) Basic research in the manufacturing of functional materials from fossil resources such as coal
- c) Upgrading technology for low-quality coal



Carbon Resource Environment

- a) Basic research in the prevention of environmental pollution
- b) Basic research in global warming and its prevention



NOVEL
CARBON RESOURCE
SCIENCES

Recruitment of Doctoral Students, Postdoctoral Researchers

This COE calls for Doctoral Students, Postdoctoral Researchers domestically / abroad.

For details:

URL: <http://ncrs.cm.kyushu-u.ac.jp>

G-COE Program Researcher Map

Program members
Carbon resource utilization cluster

Program members
Carbon resource environment cluster

Program collaborators

Collaborative member

Energy Utilization of Carbon Resources: Development of Environmentally Efficient Technology

Coal upgrading and gasification, Energy conversion

NEDO

"Innovative zero emission coal gasification electric power project"

Tsuyoshi Hirajima

Advanced processing of carbon resources; Biomass utilization

Isao Mochida

Coal gasification; Carbon materials, Carbon nanofibers

Seong-Ho Yoon

Carbon nanofibers; Reaction engineering of carbon materials

Yasutake Teraoka

Functional inorganic materials; Environmental catalytic chemistry

Jun Fukai

Thermal analysis of coal conversion; Energy saving utilization of carbon fibers

Katsuki Kusakabe

Inorganic separation membrane; Separation of environmental pollutant

Jun-ichiro Hayashi

Sustainable carbon cycle chemistry; Coproduction

Central Research Institute of Electric Power Industry, Other Universities

Ehime Univ., etc.

Koyo Norinaga

Chemical reaction engineering for carbonaceous resource conversion; Detailed simulation of chemically reacting flows

▶ P19

▶ P9

Ministry of Economy, Trade and Industry

"Advanced Education for Effective Utilization of Fossil Resources"

Kyushu society for low-carbon system

Kyushu University

G-COE, NEDO, JST, JST-MOST

Kyushu Electric Power Co., Inc.

Lignite utilization technology, nuclear power

Kyushu Bureau of Economy, Trade and Industry

Local Businesses, Other Universities

Kyushu Institute of Technology, Saga University, Kumamoto University, etc.

Advanced Technological Development for Low Energy Consuming Society

Basic chemistry

Environmental material development

▶ P23

Katsuhiko Tomooka

Organic synthetic chemistry; Efficient oxidation reaction

Hideo Nagashima

Environmentally benign chemistry; Efficient metal complex catalysts

Minoru Nishida

Transmission electron microscopy; Structure control in crystalline materials

Seong-Ho Yoon

Carbon nanofibers; Reaction engineering of carbon materials

Haruo Honjo

nonlinear physics; fractal physics

Advanced electronic material development

Shiyoshi Yokoyama

Device applications of carbon resources; Polymer photonic materials

Seigi Mizuno

Structural analysis of solid surfaces; Graphite films on vicinal SiC

Hiroki Ago

Carbon electronics; Synthesis and applications of carbon nanotubes and graphene films

Yoshiaki Takahashi

Polymer chemistry; Analysis and control of soft matters

Katsuhiko Fujita

Organic photovoltaic cells; Organic EL device

Energy material development

Michitaka Ohtaki

Thermoelectric device; Heat energy recovery

Shigeto Okada

Energy active materials and storage technology for next generation rechargeable lithium battery

Green process development

Shigeru Koyama

Heat energy conversion system; Heat transfer characteristics of CO₂

Yoshio Iwai

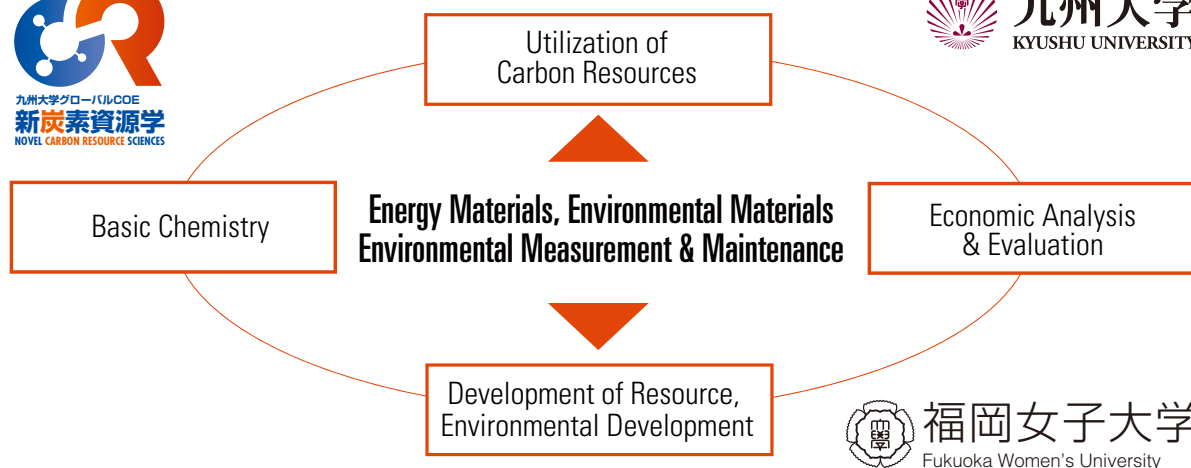
Separation technology; Supercritical fluid technology

Toshihisa Kajiwara

Polymer processing; Computer simulation

Yoshifumi Tsuge

Large scale process management; Process support system



Technology for Development of Carbon Resources

Technology for resource development below the earth

Tsuyoshi Hirajima

Advanced processing of carbon resources; Biomass utilization

Kyuro Sasaki

CO₂Storage; CO₂-ECBM; CO₂-EOR

Kikuo Matsui

Environmental restoration associated with resource development; Coal mining development and environmental issues

Hideki Shimada

Low Impact Mining; Coal Ash Utilization

Technology for resource development in the ocean

Masahiko Nakamura

Marine-viewing vehicle; Positional controls of marine constructions

Yusaku Kyojuka

Utilization of ocean energies; Simulation of marine environments

Changhong Hu

Sea keeping performance of a ship in actual seas; Simulation of ships

Environmental restoration technology

Koichiro Watanabe

Geoscience database; Environmental impact by resources development

Ryuichi Itoi

Development of geothermal energy; Development of fossil fuel resource

Keiko Sasaki

Remediation of groundwaters and soils; Reactive materials for environmental remediation

CO₂ Capture and storage (CCS)

Kyuro Sasaki

CO₂Storage; CO₂-ECBM; CO₂-EOR

Economic analysis

Nobuhiro Horii

Economic development and coal industry; China's coal and power industry

Technology for Utilization of Carbon Resources

Basic chemistry

Akira Harata

Ultrasensitive environmental analysis; Laser spectroscopic analysis

Separation, removal of pollution

Yasutake Teraoka

Functional inorganic materials; Environmental catalytic chemistry

Masaki Minemoto

Analysis of flow and transport phenomena; Upgrade of various types of plants

Economic analysis

Toshiyuki Fujita

Environmental economics; Analyses of global environmental issues

Environmental measurement

Itsushi Uno

Numerical simulation of transborder air pollution; Aerial environmental modelling in Asia

Toshihiko Takemura

Global scale simulation of aerosol

Kazuhide Ito

Chemical pollution of life environments; Indoor and environmental chemistry

Functional devices and materials for environmental concerns

Norio Miura

Sensors for environmental concerns; Electrochemical devices

Kengo Simanoe

Design of gas sensors; Development of high performance electrocatalyst

Tetsuo Hayashi

Analysis of urban thermal environment; Prediction of energy consumption in residential buildings

Tadakatsu Ohnaka

Physiological and psychological features and life environment; Research on thermo-environment and aero-environment condition

Chang-Jin Ma

Global scale air pollution; Properties of Asian dust storm particles

Optimization of CO₂ recovery using honeycomb adsorbent

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Department of Chemical Engineering, Faculty of Engineering, Kyushu University

Thermal power plants are a major contributor to anthropogenic CO₂ emissions, which have been implicated in global warming. The present study investigated CO₂ recovery from flue gases using rotary adsorption towers filled with honeycomb-type adsorbent through experiments and simulations. First, we created a simulation model to precisely estimate the performance of an actual adsorption system. The simulation estimates showed good agreement with experimental results. Furthermore, CO₂ adsorption and desorption were accurately simulated at each stage of the recovery process: adsorption, heating, purging, and cooling. Thus, the model could be helpful for system optimization in rotary-adsorption-based CO₂-recovery plants. Second, the turbulent flow in the honeycomb structure was investigated by numerical simulation using the lattice Boltzmann method. To resolve flow maldistribution inside the honeycomb structure, a new technique is proposed for automatic optimization of the pore size distribution of the porous plate placed in front of the honeycomb while keeping the total porosity of the plate constant. The technique was found to be effective in flow uniformization, especially in the case of horizontal inlet flow with an adequate inlet area.

1. Introduction

Much attention has recently been focused on global environmental conservation. CO₂ is a major greenhouse gas and so developing countermeasures against CO₂ emissions is an urgent issue. Flue gases from power plants and other fuel-burning facilities contain about 10% CO₂, making such facilities a major contributor to anthropogenic global warming. CO₂ recovery from flue gases is a promising solution to control CO₂ emission, in addition to enhancing plant efficiency. Therefore, various methods for CO₂ recovery have been studied, including absorption and desorption by alkaline fluids such as amines and K₂CO₃, adsorption by various zeolite adsorbents, and membrane separation method. Among the adsorption and desorption methods, many studies have focused on pressure swing adsorption (PSA). However, this method is impractical at the scales required for treating flue gases from actual power plants when considering the size of the vacuum pump required and the energy consumption involved. Hence, in the present study, we focus instead on another dry process, temperature swing adsorption (TSA). This process does not need a vacuum pump and, furthermore, can even run on waste heat. A conventional TSA system relies on two or more adsorption towers filled with pellets of a CO₂ adsorbent, and each is cycled through adsorption and desorption processes in alternate

shifts. However, this is not practical given the flow rates and CO₂ concentrations of the flue gasses from power plants. Therefore, this study relied on a honeycomb-type adsorbent instead, since this structure leads to lower pressure loss at large gas flow rates and allows operation with a single adsorption tower. The adsorption tower, the key component of the system, is filled with zeolite adsorbent with a honeycomb structure to prevent pressure power loss. The header sections are located at the front end of the adsorption tower and are divided into four zones: the adsorption, heating, purging, and cooling. The rotary shape allows both adsorption and desorption of CO₂ continuously using a single tower, which means that we can downsize the total system.

This paper first introduces the design method and optimization approach for the system^{1)–6)}. Next, the turbulent flow in the honeycomb structure is discussed on the basis of numerical simulation using the lattice Boltzmann method in order to resolve flow maldistribution phenomena. A new technique was proposed to automatically design the pore size distributions of the pore plate in front of the honeycomb while keeping the total porosity of the plate constant.

2. Performance analysis for CO₂ recovery

In order to achieve high performance levels, the system repeats four basic processes: adsorption, heating, purging, and cooling. During these four processes, mass and heat are transferred between the gas and adsorbent. The Basic equations describing these processes are shown in eqs. (1)–(6). These equations represent the mass balance, gas velocity, mass transfer rate, heat balance in the fluid, heat balance in the adsorbent, and adsorption equilibrium, respectively. In these equations, the temperature and adsorption distributions in the radial direction are neglected. The unknown parameters are the gas velocity u , CO₂ concentration in the gas C , equilibrium concentration C^* , adsorbed amount q , gas temperature T_g , and adsorbent temperature T_m . These are determined as functions of bed height z and time t by solving the following equations:

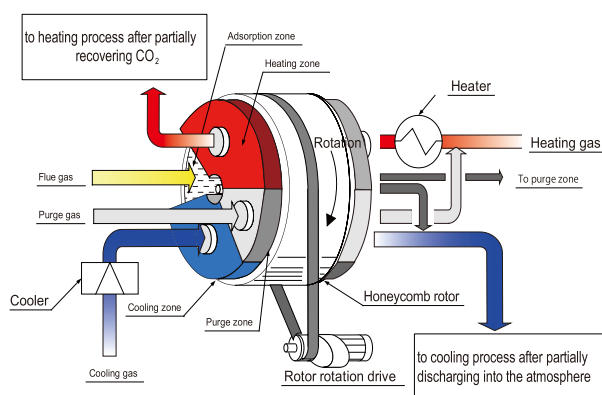


Fig. 1. CO₂ recovery system.

$$\rho_m \frac{\partial q}{\partial t} + \frac{\partial(uC)}{\partial z} = 0 \quad (1)$$

$$\rho_B \frac{\partial u}{\partial z} = -ka(C - C^*) \quad (2)$$

$$\rho_m \frac{\partial q}{\partial t} = ka(C - C^*) \quad (3)$$

$$\lambda_g \frac{\partial(uT_g)}{\partial z} = ha(T_m - T_g) - ka(C - C^*)\lambda_{gB}T_g \quad (4)$$

$$\begin{aligned} \rho_m \lambda_m \frac{\partial T_m}{\partial t} + \rho_m \lambda_B \cdot q \frac{\partial T_m}{\partial t} \\ = \rho_m Q_{ad} \frac{\partial q}{\partial t} - ha(T_m - T_g) + \rho_m \frac{\partial q}{\partial t} \lambda_{gB} T_g \end{aligned} \quad (5)$$

$$q = f(C^*, T_m) \quad (6)$$

The adsorption, heating, purging, and cooling processes were repeated until the unknown parameters settled to their steady states, allowing us to calculate the CO₂ recovery performance under various conditions.

Figure 2 compares the CO₂ adsorption amount at the start and end of each of the four processes after more than 50 repetitions. The figure illustrates that CO₂ is adsorbed by the honeycomb during the adsorption process and desorbed during the heating process. However, some CO₂ still remains in the honeycomb at the end of the heating process, as desorption process is not completed. The residual CO₂ resulted from the initial breakthrough. In addition, CO₂ is also adsorbed and desorbed in the purging and cooling system, and it is important to know the adsorption and desorption behavior in these processes.

As mentioned above, the temporal changes in the CO₂ concentration, adsorption amount, and temperature distribution in the adsorption bed are very complicated and depend on the bed height, gas flow rate, gas temperature at the inlet, divided angle of each zone, and the revolution speed of the rotary. These control parameters must be optimized.

Next, the evaluation results of the system under some conditions are shown. The typical evaluation parameters include the CO₂ recovery rate and energy consumption. The CO₂ recovery rate is defined as the ratio of the quantity of CO₂ actually recovered to the total quantity of CO₂ in the flue gas. The energy consumption is defined as the energy required in the heating process to recover 1 kg of CO₂. In order to optimize the system, the energy consumption should be minimized while the CO₂ recovery rate is kept at the target value. The simulation conditions are listed as follows. The constant parameters are:

Diameter of the adsorption tower: 14.5 m

Bed height of the tower: 0.5 m

Flow rate of flue gas: 14,000 m³(STP) · h⁻¹

CO₂ concentration in flue gas: 13.5%

Flow rate of cooling gas: 93,000 m³(STP) · h⁻¹

Flow rate of purge gas: 800 m³(STP) · h⁻¹.

The parameters adjusted include the desorption gas temperature, CO₂ concentration in the desorption gas, and the flow rate of the desorption gas.

Figure 3 shows the CO₂ recovery rate and the energy consumption as functions of the desorption gas temperature. Although the CO₂ recovery rate improved as the desorption gas temperature increased, the rate of the increase reduced at 450 K. However, consumption energy reached a minimum point at a desorption gas temperature of 423 K. This is because desorption was slow at the lower temperatures, whereas heating energy was wasted at the higher temperatures. Therefore, the optimum desorption

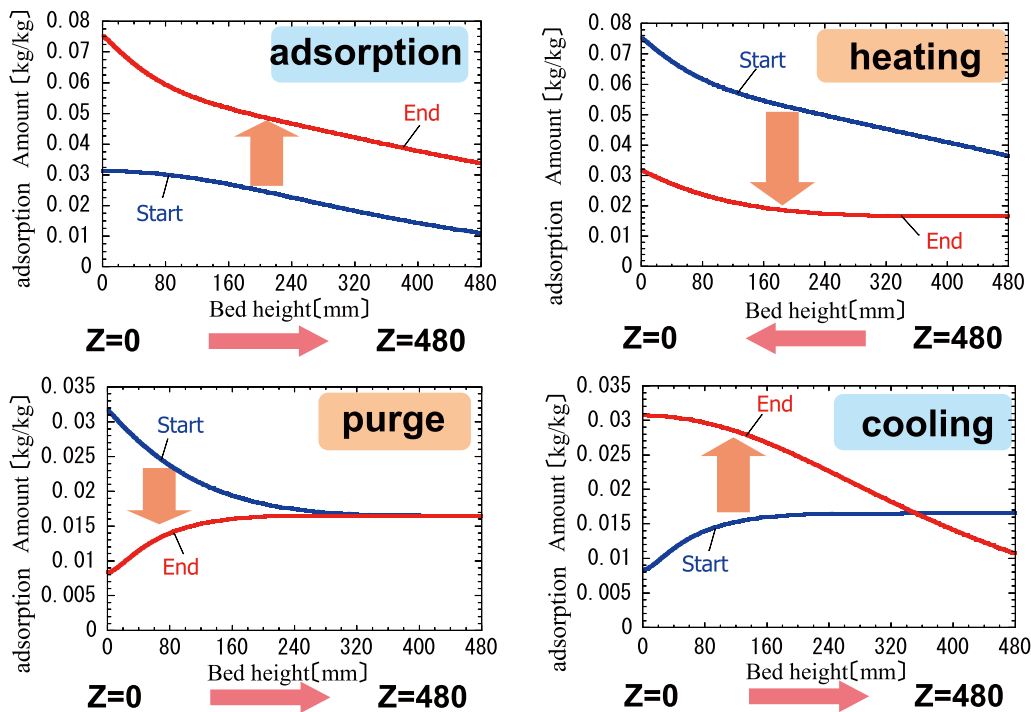


Fig. 2. CO₂ adsorption amount at the start and end of each of the four processes.

gas temperature is 423 K. The CO₂ recovery rate was approximately 77% at this temperature.

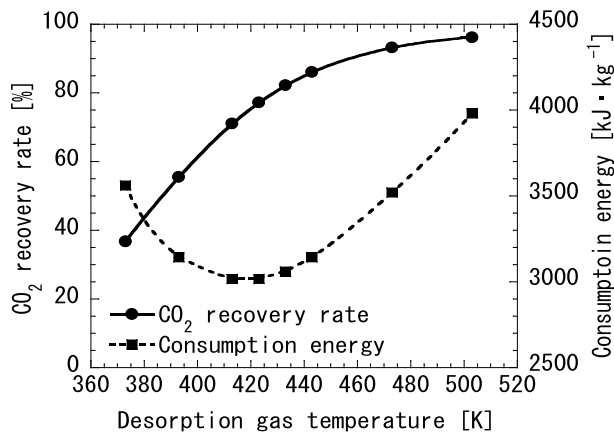


Fig. 3. Relationship between CO₂ recovery performance and desorption gas temperature.

3. The proposed system

Here we describe the design concept for the actual proposed system for recovering CO₂ from flue gas at a flow rate of $1.80 \times 10^6 \text{ m}^3(\text{STP}) \cdot \text{h}^{-1}$. The size of the actual plant was estimated from the results noted above. Figure 4 shows a schematic illustration. The total height will be about 26 m and comprise 26 vertically stacked absorber rotors (diameter, 14.5 m; bed height, 0.5 m).

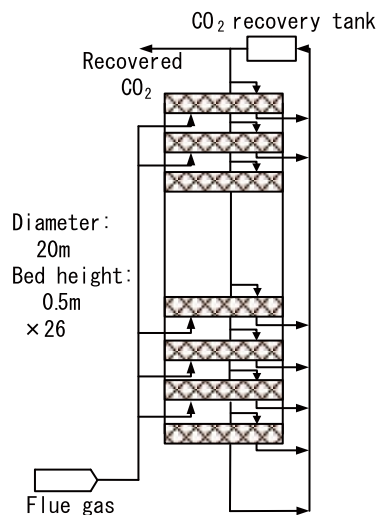


Fig. 4. Schematic of actual system.

4. Flow distribution in the honeycomb structure

The zeolite-type adsorbent with the honeycomb structure in the adsorbent tower is the key novelty of the proposed system in order to reduce pressure loss. However, this characteristic of low pressure loss often causes flow maldistribution in the honeycomb structure. Although the pellet-type adsorbent has large pressure loss, it acts as a dispersing agent. However, the honeycomb structure often causes flow maldistribution, which often causes not only decreased performance but

also decreases the durability of the total system because of cracking by thermal stress. In order to prevent these defects, flow distribution in the honeycomb must be made uniform, for example, by using baffle plates to reduce the hydrodynamic pressure of the inlet gas. The inlet gas is introduced in the opposite direction to the honeycomb, and porous plates are placed in front of the honeycomb in other instances. However, these effects have not been always qualitatively known.

To understand the flow distribution problem inside the honeycomb structure, the turbulent flow in the honeycomb structure was numerically simulated by the lattice Boltzmann method (LBM)⁷⁾. On the basis of this, a new technique is proposed to automatically optimize the pore size distribution of the pore plate placed in front of the honeycomb while keeping the total porosity of the plate constant.

The computational domain is shown in upper panel of Figure 5. The honeycomb size is 480×100 lattices in width and height, respectively, and the honeycomb has 40 channels each with a width of 10 lattices. The flow is introduced from the bottom left and changes its direction toward the honeycomb at the header section of the system. A porous plate with N pores of an equal distance apart is placed in front of the honeycomb. This flow pattern is often used when the total height of the system is limited.

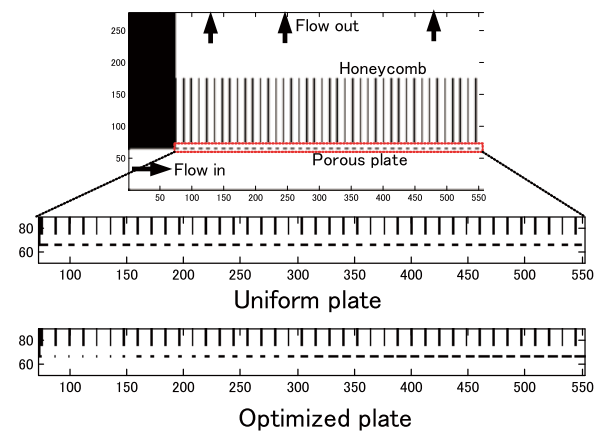


Fig. 5. Computational domain and shape of porous plate before and after optimization.

While the flow in the system is calculated by LBM, the pore diameter of the porous plate most connected with the channel with the maximum flow velocity is small at a constant time interval, and the pore diameter of the porous plate most connected with the channel with the minimum flow velocity is large. The specific procedures are listed below.

- After the flow reached a steady state, virtual particles with no mass are released from the pores of the porous plate. The virtual particles have information regarding the pores from which they were released.
- The mean velocity in each channel is calculated to determine the channels with the maximum and minimum velocities.
- The pore diameter of the porous plate connected

with the channel with the maximum flow velocity is small. On the other hand, the pore diameter of the porous plate most connected with the channel with the minimum flow velocity is large.

After repeating procedures A to C, it is expected that the pore diameter automatically changed while keeping the total porosity constant so as to afford uniform flow through the honeycomb channels. The two-dimensional simulation was conducted at a Reynolds number of 60,000. The maldistribution is evaluated by the coefficient of variance defined in eq. (7).

$$C_v = \frac{1}{u_m} \sqrt{\frac{1}{N} \sum_{i=1}^N (u_i - u_{ave})^2} \quad (7)$$

where u_i is the mean velocity in the i -th channel and u_{ave} is the mean of these values. A smaller coefficient of variance indicates a more uniform flow, and the flow is completely uniform when C_v equals zero. The time variation of C_v is illustrated in Fig. 6. Until time step τ reached 15,000 steps, the shape of the porous plate was kept constant. After that, optimization was started and ended at $\tau = 150,000$. Figure 6 shows that after $\tau = 20,000$, C_v gradually began decreasing from 0.7–0.8 before the optimization to a constant value of 0.3 after $\tau = 60,000$. The proposed optimization method seems to work well between $\tau = 20,000$ and $\tau = 60,000$. Although the value of C_v slightly increased after the optimization, it retained a value of 0.35.

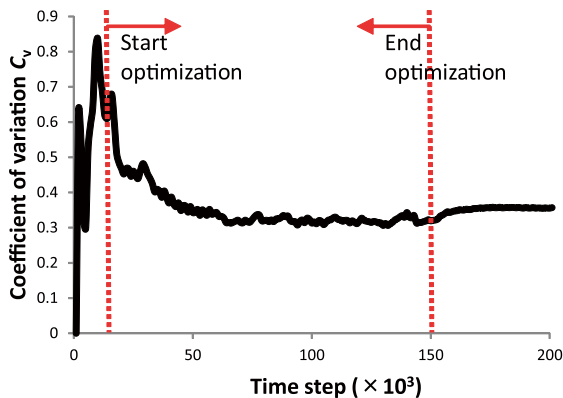


Fig. 6. Time history of coefficient of variation.

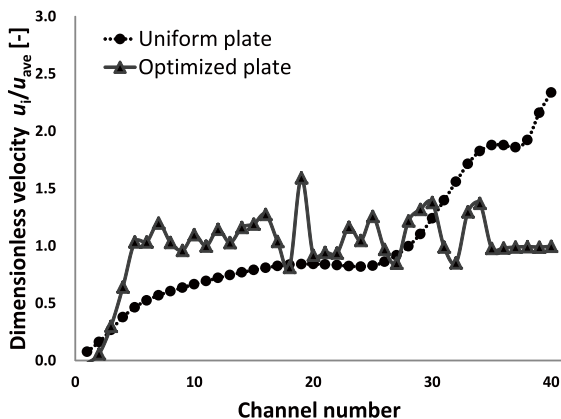


Fig. 7. Comparison of mean velocity in each channel with uniform and optimized plates.

The comparison of mean velocity in each channel with uniform and optimized plates is shown in Fig. 7. In the case of uniform plate, it seemed there was no flow in the channels near the gas inlet, while most gas flowed on the opposite side of the gas inlet because of the hydrodynamic pressure. The value of C_v was 0.7. In the case of the optimized plate, uniformization of the velocity distribution was achieved and the value of C_v decreased to 0.35.

5. Conclusion

Numerical simulations of a CO₂ recovery system were conducted in order to determine the optimal operation conditions for an actual plant. Thermal swing adsorption (TSA) was adopted for rotary adsorption towers filled with honeycomb-type adsorbent. It was shown that the CO₂ concentration in flue gases could be reduced by up to 90%, with a recovery rate of more than 60%, with the proposed system. However, in order to put the system into practical use, it is important to reduce energy consumption further, for example, by using more efficient adsorbents and effectively exploiting waste heat.

Next, to understand the flow maldistribution phenomena inside the honeycomb structure, the turbulent flow in the honeycomb structure was numerically simulated by the lattice Boltzmann method. On the basis of this, a new technique was proposed to automatically optimize the pore size distribution of the pore plate placed in front of the honeycomb while keeping the total porosity of the plate constant. As a result, this technique affected flow uniformization, especially in the case of a horizontal inlet with an adequate inlet area. The proposed technique also showed that the coefficient of variation, which represents the uniformity of the flow velocity, could be reduced to 0.3–0.4.

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Development of nanocarbon research for future electronic applications

Hiroki Ago

Institute for Materials Chemistry and Engineering, Kyushu University and PRESTO-JST

There is growing interest in “nanocarbon materials”, mainly carbon nanotubes and graphene, for future electronic applications, such as transistors, sensors, and integrated circuits. The realization of these electronic applications require precise control of the structure as well as their integration. In this article, our recent progress of horizontally aligned single-walled carbon nanotube growth and epitaxial growth of single-layer graphene is reviewed. Growth mechanism and device properties are also demonstrated.

1. Introduction

Recently, research on flexible electronics based on π -electrons of carbon atoms, which is represented by organic electronics, has attracted a great interest. However, organic materials suffer from low carrier mobilities less than $10 \text{ cm}^2/\text{Vs}$, which is much lower than those of silicon (mobilities of electron and holes are 1500 and $450 \text{ cm}^2/\text{Vs}$, respectively). The low mobility of organic materials is mainly ascribed to the carrier hopping between organic molecules or polymers.

Single-layer graphene (SLG), two-dimensional honeycomb-lattice carbon network with single atom thickness, and single-walled carbon nanotube (SWNT), one-dimensional cylinder rolling up a graphene sheet, are called as “nanocarbon materials” (Figure 1). These nanocarbon materials show extraordinary high carrier mobility (up to $200,000 \text{ cm}^2/\text{Vs}$). This high mobility is important not only for high speed operation of electronic devices but also for low-energy operation devices by suppressing heat emission. Furthermore, nanocarbon materials are consisting of carbon atoms which are widely available resource, and they show high chemical stability and mechanical flexibility.

For industrialization of these nanocarbon materials to future electronics, their integration on a substrate and controlling their electronic structure are required. In this article, we review our current progress on the controlled growth of SWNT and SLG based on chemical vapor deposition (CVD) using transition metal catalysts.

2. Horizontally aligned nanotube growth

SWNTs have well-defined one-dimensional structure with a nanoscale diameter ($1\text{--}3 \text{ nm}$), which is much smaller than line patterns made by modern lithography techniques¹⁾. In addition, because SWNTs show high carrier mobility and stability, electronic applications like field-effect transistors (FETs) and transparent electrodes are expected. There are two possible directions in their applications; (i) application to large-area flexible devices and (ii) integration with modern Si electronics. Horizontal alignment of SWNTs on a substrate is essential to increase the operation current and also to apply the gate voltage to all the nanotubes in a channel. The direct growth of SWNTs on a substrate by CVD can offer surface-clean SWNTs with low defects. The CVD method is also advantageous in terms of large-scale integration on a substrate.

In the CVD growth of SWNTs, a fast gas flow and an electric field have been applied to horizontally align SWNTs on a substrate, but their density and the degree of alignment were not sufficiently high. We discovered the horizontal alignment of SWNTs on sapphire ($\alpha\text{-Al}_2\text{O}_3$) substrates with r- and a-planes²⁾. Figure 2a,b shows scanning electron microscope (SEM) images of the SWNTs grown on sapphire and SiO_2 substrates. It is clearly seen that the randomly oriented tubes grow on a SiO_2 substrate, while the horizontal alignment occurs on a sapphire r-plane.

Because the SWNTs are aligned along a specific crystallographic direction ($[1\bar{1}0]$ direction for r-plane) and no alignment is seen on highly symmetric c-plane sapphire, we conclude that anisotropic van der Waals interaction between SWNT and sapphire surface gives the nanotubes' horizontal alignment. We call this substrate-restricted growth as “atomic arrangement-programmed (AAP) growth”. It is noted that the pre-defined direction of SWNTs greatly improves the fabrication yield of nanotube devices. The nanotubes aligned on sapphire substrates were confirmed to be single-walled nanotubes from resonance Raman spectroscopy. So far, only sapphire and quartz (SiO_2) crystals offer the horizontal alignment due to their anisotropic surface structures and chemical/thermal stability.

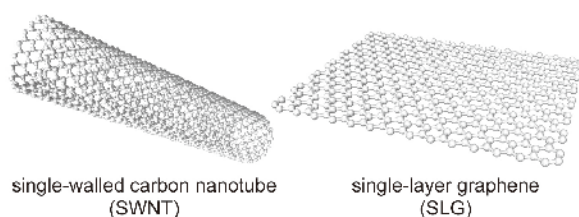


Fig. 1. Structures of nanotube and graphene.

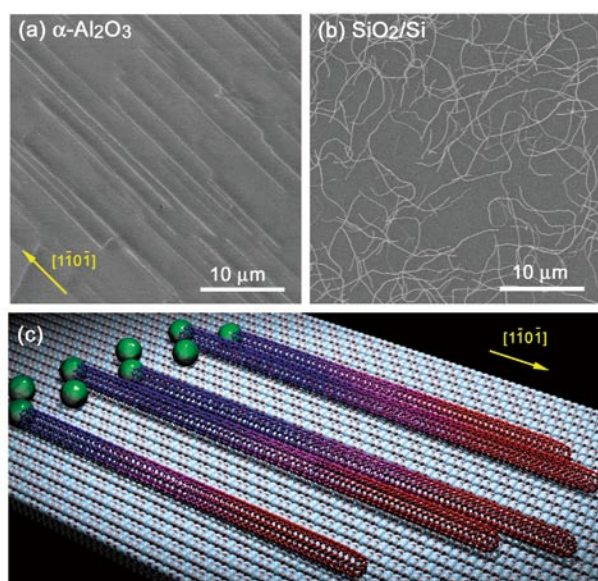


Fig. 2. SEM images of SWNTs grown on r-plane sapphire (a) and silicon (b) substrates. The nanotubes appears thick due to charging, but the actual diameter is about 1-2 nm. (c) Illustration of the horizontally aligned SWNTs grown on sapphire surface.

3. Alignment mechanism

For the growth of SWNTs, transition metal nanoparticles (green particles in Fig. 2c) and hydrocarbon gas are used as catalyst and carbon feedstock, respectively. Carbon atoms, catalytically decomposed on the metal surface, are organized into nanotube structure with π -conjugated network via precipitation from the metal nanoparticles. Through the appropriate patterning of the catalyst, the control of the position of aligned nanotubes was realized. As shown in Figure 3, the highly aligned SWNT array is obtained from the stripe catalyst pattern. The aligned SWNTs have the length longer than 100 μm , indicating a very high aspect ratio ($>10^5$) and high degree of alignment. The patterning can avoid the contamination of the sapphire surface so that the highly aligned and very long nanotubes were obtained.

Two growth modes are plausible for the catalytic SWNT growth. One is “tip-growth” mode, in which catalyst nanoparticle stays at the tip of a SWNT, thus moving forward as the nanotube grows. Another is “base-growth” mode, in which the catalyst stays at the base (root) of the nanotubes during its growth. Investigation of the growth mechanism is important not only for understanding of the alignment mechanism, but also for future control of nanotube structure. We tried to clarify the growth mode in the horizontally aligned SWNTs by isotopically labelling the carbon atoms. In the CVD, the carbon feedstock was switched from $^{13}\text{CH}_4$ to $^{12}\text{CH}_4$ to introduce a spatial distribution of $^{13}\text{C}/^{12}\text{C}$ isotopes along the SWNT axis. Raman mapping measurement was performed for the isotope-labeled SWNTs, as the phonon frequency changes with mass of C atoms. We found that

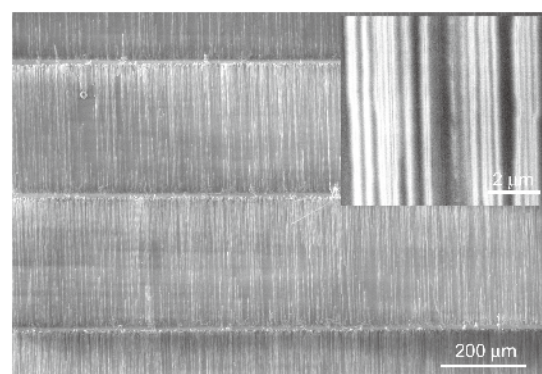


Fig. 3. SEM image of horizontally aligned SWNTs grown from the patterned catalyst (white horizontal lines). Inset shows a high-magnification image.

^{13}C , which is introduced at the beginning of the reaction, is enriched at the nanotube tip, while ^{12}C is enriched at the base of the nanotube⁴. This result clearly indicates that the aligned SWNT is grown based on the “base-growth” mode, thus suggesting the importance of SWNT-sapphire interaction on the alignment^{4,5}.

Effects of a surface step-terrace structure on the SWNT alignment are also interesting. We studied a-plane sapphire substrates with clear step-terrace structure. The step height and direction were controlled by the miscut angle and annealing condition. It was found that SWNTs align along a specific crystallographic orientation when the step height is low (0.2-0.3 nm). When the step height was higher than 0.3 nm (double and triple atomic steps), SWNTs changed the growth direction so as to align along the step edges⁶. This result suggests that there are two alignment mechanisms in the horizontally aligned SWNTs, that is lattice-oriented and step-templated growth. Recently, we demonstrated orthogonally aligned SWNT arrays by combining these two mechanisms⁷.

4. SWNT transistors

Our horizontally aligned growth of SWNTs with pre-defined direction greatly contributes the yield of device fabrication process. Figure 4a shows an SEM image of an individual SWNT bridging between two adjacent Au electrodes. The SWNT devices showed two different gate voltage dependences; one is strongly dependent on the gate voltage (Fig. 4b), another is independent of the gate voltage with relatively high current (Fig. 4c). The former is a field-effect transistor (FET) made from a semiconducting SWNT, showing high on/off ratio of 10^4 - 10^5 . In this device, one SWNT shows the on current of several μA . The gate voltage independent device (see Fig. 4c) is originated in metallic SWNT. Statistically, 60-70% of the aligned SWNTs were semiconducting, while 30-40% were metallic, indicating the mixed growth of semiconducting and metallic tubes even on the sapphire surface.

We further studied chirality of the horizontally aligned SWNT by photoluminescence (PL) spectroscopy. The

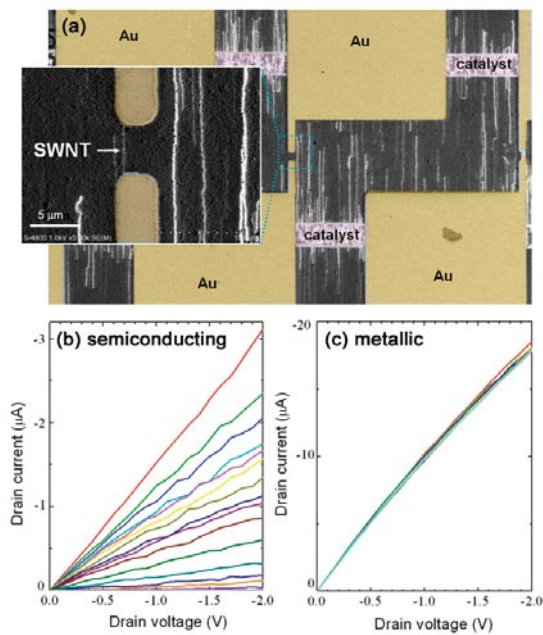


Fig. 4. SEM image of a SWNT-FET fabricated on sapphire r-plane. I_d - V_d curves obtained for semiconducting (b) and metallic (c) SWNTs measured with different gate voltages.

nanotube chirality is defined as the diameter and wrapping angle of a graphene sheet¹¹. Our PL measurements indicated the possible chirality-selective growth of SWNTs depending on the crystalline plane of sapphire⁸. On r-plane sapphire, armchair type structures were dominant, while zigzag type was dominant on a-plane. Because it is widely recognized that as-synthesized SWNTs have mainly armchair structure, the zigzag structures obtained on a-plane is interesting. This finding is expected to develop to the selective growth of SWNTs for future electronic applications.

5. Controlled growth of graphene

Graphene has attract a great interest since the first preparation of SLG in 2004⁹. For the large scale synthesis of graphene with low cost, much research effort has been devoted to the CVD growth from the end of 2008. A graphene film is precipitated on a metal catalyst film with 200-1000 nm thickness from methane feedstock at high temperature (900-1000 °C). Most of the CVD research works so far have employed a metal film deposited on a silicon substrate (SiO_2/Si) as catalyst. However, as the silicon substrate has amorphous surface layer (SiO_2), the catalyst metals films usually have a polycrystalline structure.

We tried to prepare a crystalline metal film epitaxially deposited on single-crystalline substrates and apply to a catalyst for the graphene growth. Very recently, we succeeded in the growth of uniform SLG over the epitaxial Co and Cu films^{10,11}. Although it was believed that transition metals with high carbon solubility, such as

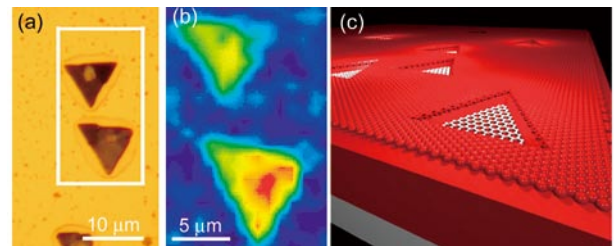


Fig. 5. (a) Optical microscope image of triangular pits appeared on Co film surface. (b) Raman mapping image of the graphene formed inside the pits. (c) Schematic of the graphene formation inside the pits.

Ni and Co, cannot give uniform graphene film, we first achieved the uniform single-layer graphene by using epitaxially deposited crystalline Co films. Furthermore, due to the epitaxial metal film, the orientation control of hexagonal network of graphene is demonstrated for the first time^{10,11}. The uniform and orientation controlled graphene films are interesting in terms of growth mechanism and electron transport properties, and current study is underway.

When thin films of the epitaxial metal were used as catalyst, a number of pits appeared on the metal surface. We found that graphene is preferentially formed inside these pits, as depicted in Figure 5. The pit structure, in other words, graphene shape can be triangular or rectangular depending on the crystalline substrate. This finding is interesting in terms of self-assembled growth of graphene.

6. Future prospect

The horizontal alignment of SWNTs should become an essential technique for integration of a large number of SWNTs for nanoelectronic applications. Actually, Rogers and coworkers have demonstrated the operation of a radio using aligned SWNTs grown on quartz substrates as a circuit¹³. Transfer of the aligned SWNTs to transparent and flexible substrates has been also demonstrated, which can be developed to flexible electronics¹⁴. However, the transfer process as well as single crystalline substrates have several problems in terms of cost and time consuming transfer processes. In particular, large scale integration (LSI) application requires the integration on silicon wafers. Recently, we realized the horizontal SWNT alignment even on the silicon substrate by creating artificial trench structures on the substrate surface^{15,16}. Future development of selective growth of SWNTs with unique chirality or electronic structure is demanded to commercialize nanotube devices.

Research on graphene has just started from 2004, and there are many possibilities in the graphene research. Unique applications as well as interesting physical properties are expected based on its ideal two-dimensional structure. Through the controlled growth of nanocarbon materials, we believe that "carbon electronics" opens up a

new stage for real applications.

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Research Report

Development of Mechanisms on Primary Reactions during Coal Volatile Combustion: Numerical Investigation

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This research report resumes the results of research work for developing reaction mechanisms during coal volatile combustion based on our related publications. Developments of coal conversion become more familiar in the worldwide at the present. Computational Fluid Dynamics (CFD) plays a key role to explain these developments of different coal chemistry steps including devolatilisation, volatile combustion and reforming, char oxidation and char gasification. In the research work, firstly, the authors develop the reduced mechanism that has a good agreement with the mechanism model of primary reaction of coal volatiles that consists of 255 chemical species and 1095 elementary reactions. Secondly, in the viewpoint of nowadays environmental issue for CO₂ reduction, carbon resource utilization especially how to increase syngas during coal gasification, the authors investigate continuously the primary reactions of coal volatiles including the soot formation mechanism for O₂/CO₂ environment to analyze the combustion components. The effects of CO₂ concentration, reaction temperature and pressure are also discussed in this research report for the soot model that provides a better result of the increase in product concentrations of CO, H₂ and the reduce in CO₂.

Keywords: reaction mechanism, reduced mechanism, soot formation, aromatics, coal volatiles, plug flow reactor.

Introduction

As well known that coal has a potential energy value, the substantial worldwide attention is being focused on cleaner and more efficient use of coals. Coal gasification process, in particular, allows an efficient use of this energy source with a low environmental impact. Continued utilization of coal is depending on the availability and development of the new process. Presently, about 40% of electric power generation in the world depends on coals.

As coal heats up, the volatile components of the coal will diffuse into the gas stream. Volatiles generally are composed of H₂, H₂O, CO, CO₂, hydrocarbon gases, hydrocarbon liquids, and polycyclic aromatic hydrocarbons (PAHs). Most of the compounds will continue to react to produce successively lighter gases as the more complex molecules decompose, eventually forming CO₂ and H₂O provides if the sufficient oxygen is available. PAHs are products of primary pyrolysis and PAHs are precursors of soot in secondary pyrolysis. The conversion of PAHs into soot during secondary pyrolysis is accompanied by release of CO and H₂.

New advance in instruments, computers and numerical methods have greatly increased in order to conduct the research efforts in coals. In this numerical research work, the authors divide the study into two parts¹⁻³. One is to develop a numerical model that is validated with the experimental results and then to make a reduced model for CO₂ gasification that shows similarity with primary mechanism consists of 255 chemical species and 1095 elementary reactions⁴. The reduced model contains 53 chemical species and 73 elementary chemical reactions and the comparison between the primary and reduced mechanisms is provided. The second part is to extend the previous work for developing mechanism including the soot formation. The reaction mechanism consists of 276

species and 3793 reactions⁴). The comparison between soot formation and without soot models is also provided. Moreover, the effects of CO₂ concentration, temperature and pressure for the appropriate soot model are also reported in this paper.

Mathematical Model

A plug flow reaction model for reaction of coal volatiles is developed for O₂/CO₂ gasification. The model is numerically developed using the input data of coal volatile pyrolysis that has concentration of H₂, CO, CH₄, O₂ and CO₂ of 0.00049, 0.00283, 0.00211, 0.00729 and 0.02241 in mass fraction, respectively. Simulation is conducted inside the reactor of 28 mm in diameter and 1200 mm in length. The plug flow reactor model can be used to model multiple reactions as well as reactions involving changing temperatures, pressures and densities of the flow. In the ideal tubular reactor, which is called the plug flow reactor, there is assumed to be complete mixing perpendicular to the direction of flow (i.e. the radial direction) and no mixing in the direction of flow. In the plug flow, the residence time in the reactor is the same for all elements of fluid. It means that the reaction proceeds as the reactants in a plug progress along the reactor tube. There is ideally no back-mixing in the reactor and there exists a uniform temperature, pressure and velocity profile across the radius.

All the gas phase and surface phase reactions are considered in this mathematical model are as follows:



The lower case letters (*a*, *b*, *c* and *d*) represent

stoichiometric coefficients, while the capital letters represent the reactants (*A* and *B*) and the products (*C* and *D*).

k is the proportionality constant called the specific rate coefficient for the above reaction and follows the Arrhenius equation.

$$k = A_f T^\alpha \exp^{\frac{-E}{RT}} \quad (2)$$

where A_f is a frequency factor (mole-m-sec-K), T is temperature (K), α is temperature exponent, E is activation energy (J/mole) and R is the gas constant (J K⁻¹ mole⁻¹).

Reduced Mechanism

The aim of this study is to reduce the number of species and reactions to get a reduced mechanism small enough to use in CFD calculations. There is no theoretical limitation of the number of species utilized in the mechanism calculations however the simulation time becomes unacceptably long. There is no species limit in Chemkin-CFD, but the practical 50 species limit was introduced in the code of Fluent. Species entering the combustion process and the resulting stable products of the reaction process are selected as important species.

The authors first consider only five compound species (H₂, H₂O, CO, O₂, and CO₂) that is obtained by filtering the species based on the mass fraction. Then the Rate of Production (ROP) analysis has been studied. ROP analysis is particularly useful for plug-flow systems, where the computational expense for the added calculations is small and it is possible to consider data from a large reaction set. ROP analysis determines the contribution of each reaction to the net production or destruction rates of a species. The percentage of the contribution of the *i*-th reaction to the formation of or consumption, C_{ki} of a species *k* is calculated as:

$$C_{ki} = \frac{\omega_{ki}}{\omega_k} \times 100 \quad (3)$$

where ω_k is the net molar production rate per unit volume of the *k*-th species.

The authors successively consider the most dominant reactions for each species and make a new mechanism. Then, the size of the mechanism is gradually increased by adding the chemical species and number of dominant reactions, and the procedure is terminated when the deviation becomes smaller. The reactions are added or removed to modify the reduced mechanism by temperature sensitivity analysis. The resulting mechanism has 15 compound species and 73 elementary chemical reactions that include 37 intermediate species¹⁾.

Reaction Mechanism including Soot Formation

Nucleation is the process of forming new condensed-phase particles from a continuous phase, such as gas

and vapor. Particle nucleation is the most important step in soot formation and results in generation of the solid particles. It is irreversible and all reactants must be gas phase species. The PAH molecules first grow into planar molecules while simultaneously reacting with the gas phase species and colliding with other PAH molecules to form large molecules. The PAH compounds having large molecular mass about 2000 is considered soot and the reaction mechanism is described from benzene to coronene (C₂₄H₁₂). Then, considering the concentration of H₂, CO, CO₂ and soot in the outlet of the reactor the authors define which model has significant regarding energy and environmental issue.

This soot model consists of the following principal processes: initial aromatic ring formation during small hydrocarbon oxidation, formation of larger PAH, particle nucleation/inception through coalescence of PAHs, particle growth and particle oxidation. Particle oxidation produces the lower PAHs. The reaction mechanism developed in this model consists of 276 species, 2158 conventional gas phase reactions and 1635 surface phase reactions⁴⁾. Based on the detection of compounds containing up to 160 carbon atoms is considered as a particle⁵⁾, the remaining all aromatic compounds are considered as PAHs in this soot model. The main reactions considered in this model are:



where * indicates a radical entity.

Results and Discussion

Reduced Mechanism

The reduced mechanism is tested against the primary mechanism. The comparison of the two mechanisms can be seen in Fig. 1 that shows the concentration profiles of the major combustion species (H₂, CH₄, H₂O, CO and CO₂).

The Fig. 1-a shows the result when the authors consider 10 compound species of H₂, CH₄, H₂O, C₂H₄, C₃H₆, CO, CO₂, O₂, C₆H₆ and chrysene. The concentration difference between primary mechanism and reduced mechanism for H₂O and CO is large. But, when we consider 15 compound species of H₂, CH₄, H₂O, C₂H₄, C₂H₆, C₃H₆, C₄H₈, C₃H₈, CO, CO₂, O₂, C₆H₆, C₇H₈, C₆H₅OH and chrysene, then the result provides the smaller difference for all major combustion species as shown in the Fig. 1-b. This good agreement mechanism has 15 compound species and 73 elementary chemical reactions that include 37 intermediate species.

This reduced model shows good results when the temperature and pressure are maintained up to 1373K and 1.0 MPa, respectively¹⁾.

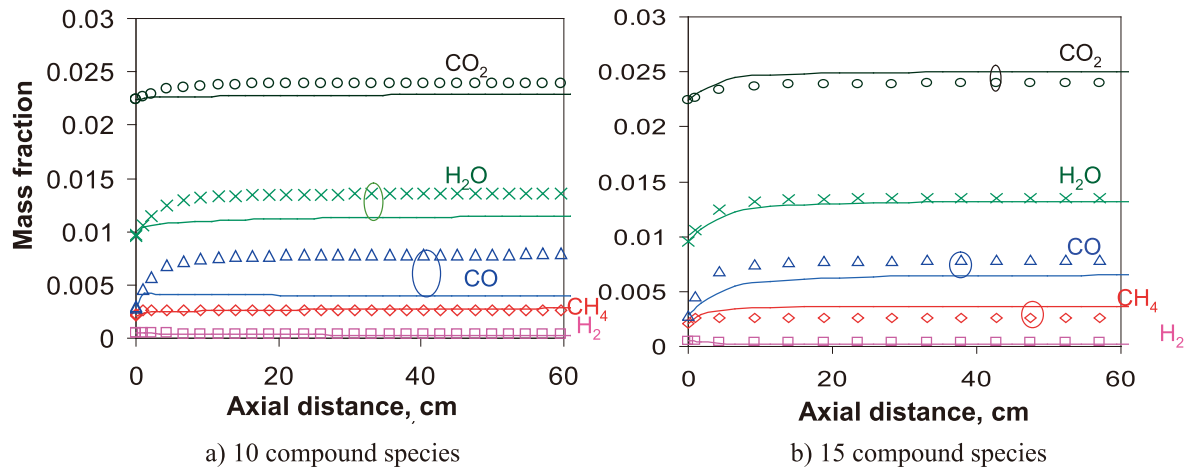


Fig. 1. Comparison between the primary mechanism (symbol) and the reduced mechanism (solid line) at 1273 K, 0.1 MPa.

Reaction Mechanism including Soot Formation

It is seen in Fig. 2-a that the both soot and without soot models provide different concentration profiles for all major combustion species. The concentration of CH_4 decreases for soot model since it is a source of PAHs in order to form the soot. The increase in concentrations of H_2 and CO in the soot model is due to the formation of CO and H_2 from the oxidation of soot. As illustrated in the Fig. 2-b, the significant difference of PAH concentration is occurred for between the soot and without soot models. The PAHs concentration for the soot model decreases since a number of PAHs produces the soot. The soot is almost zero at this condition.

Temperature study (1273–1873 K) has been investigated at constant pressure of 0.1 MPa. It is seen in the Fig. 3 that the product concentrations of H_2 and CO become large when the reaction temperature increases. The reduction of CO_2 concentration is significant at high temperature. This is mainly due to the decomposition of CO_2 to CO and radical oxygen. Furthermore, the oxidation of PAHs occurs in order to produce more concentrations of CO and H_2 at higher reaction temperature. In the result, the product concentration of PAHs decreases with increasing the reaction temperature. It is also seen in the Fig. 3-d that the concentration of PAHs intensively drops from initial condition for forming soot.

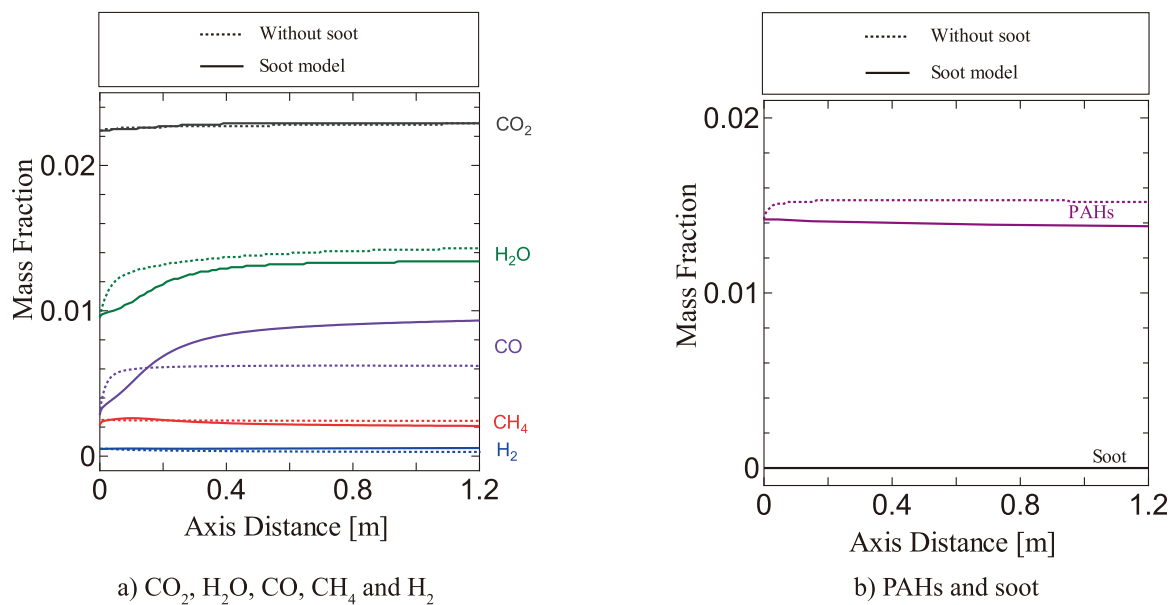


Fig. 2. Comparison between the mechanism with soot and without soot at 1273 K, 0.1 MPa.

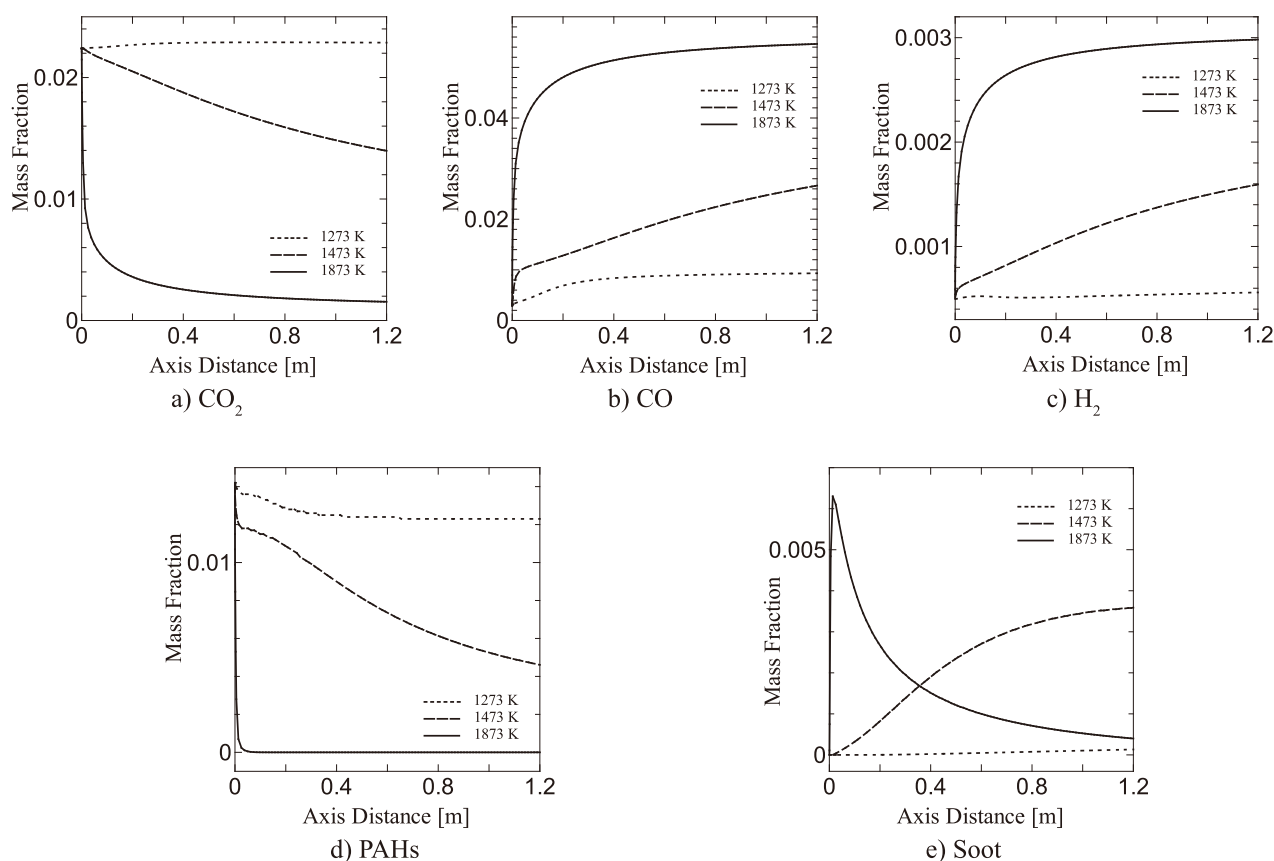


Fig. 3. Concentration profiles along the reactor at 0.1 MPa with various reaction temperatures.

Fig. 4 shows concentration profiles for the soot model along the axial position of the reactor at 1473 K, 0.1 MPa with various initial CO₂ concentrations until ten times from initial input of 0.02241 in mass fraction. As illustrated in the Fig. 4, the soot model provides the better results at higher CO₂ concentration for increasing significantly the product concentration of CO and decreasing the soot. Although soot reduces with increasing CO₂ but still there are more PAHs and soot exist in the outlet of the reactor at temperature 1473 K.

From the Fig. 5, at temperature 1473 K CO₂ concentration has not yet provided the more significant effect. But, at high temperature (1673-1873 K) CO₂ makes significant effect on PAHs as well as soot. From this discussion, it means that to get significant effect from CO₂ concentration, the temperature should be maintained at high temperature about 1673 K due to decomposition of CO₂. At higher temperatures CO₂ have large effect on soot and PAH reduction. On the other hand, O₂ shows good prediction of soot and PAHs at lower temperature³.

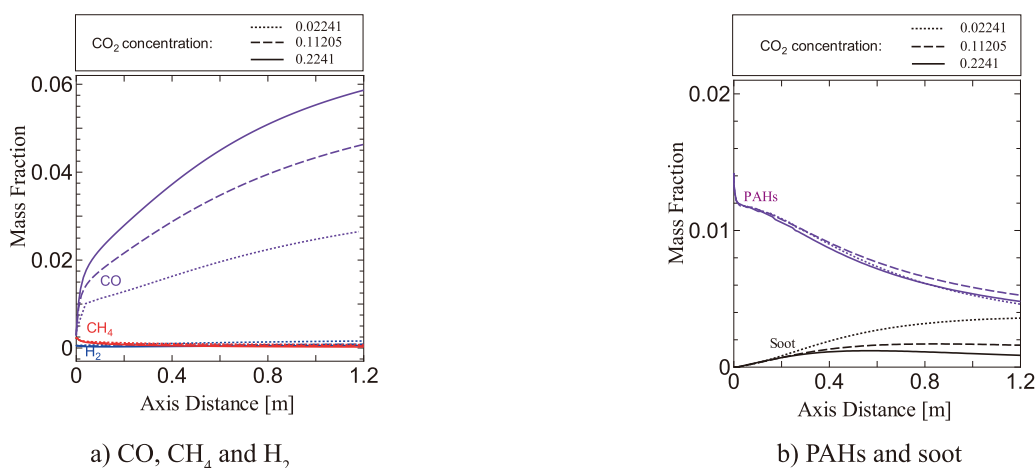


Fig. 4. Concentration profiles at 1473 K, 0.1 MPa with various CO₂ input.

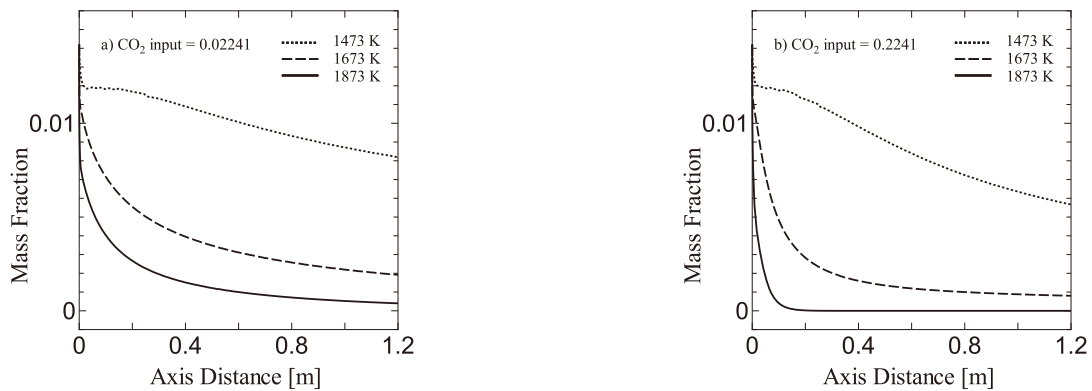


Fig. 5. Concentration profiles of total of PAHs and soot compound at 0.1 MPa with various temperatures.

Fig. 6 shows the effect of reaction pressure on product concentrations. The concentrations of H_2 and CO become high when the pressure increases, but the concentrations of CO_2 and PAHs reduce. In the view point of reduced CO_2 and high products of CO and H_2 , the reaction temperature and pressure should be maintained at high condition for soot model^{2, 3}. Formation of aromatics decreases with increasing the reaction temperature and pressure.

Conclusions

The numerical research work for developing reaction mechanisms during coal volatile combustion has been investigated. The reaction mechanism (255 species and 1095 elementary reactions) can be reduced substantially by using the rate of production analysis to a reduced mechanism (53 chemical species and 73 elementary chemical reactions). This reduced model shows good

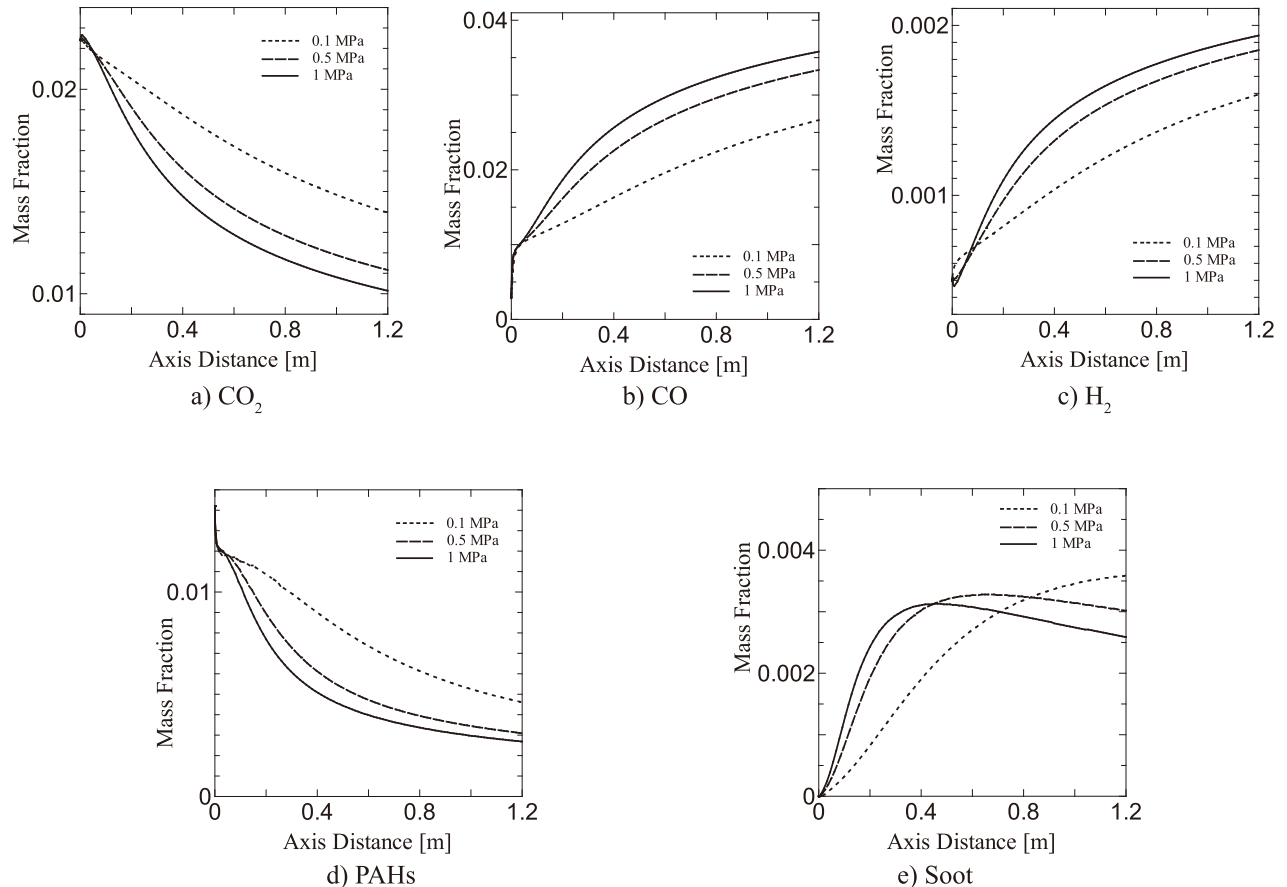


Fig. 6. Concentration profiles along the reactor at 1473 K with various reaction pressures.

results when the temperature and pressure are maintained up to 1373 K and 1.0 MPa, respectively.

The soot formation model on primary reactions of coal volatiles in a plug flow reactor for O_2/CO_2 environment also has been numerically investigated. Providing the calculated data of simulation model is to predict concentration profiles of the major combustion species and PAHs. When increasing the reaction temperature, the product concentrations of CO and H_2 become high. Considering the advantages of the increases in CO, H_2 and the decreases in soot, the effect of CO_2 concentration are observed and discussed for the soot model at higher temperature. CO and H_2 also increase with increasing the reaction pressure. Furthermore, the CO_2 and PAHs reduce at the both higher temperature and pressure conditions. At higher temperatures CO_2 have large effect on soot and PAH reduction, but O_2 shows good prediction of soot and PAHs at lower temperature.

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ACTIVITY REPORT

Interim Report of Student Forum on Novel Carbon Resource Sciences

Professor, Institute for Materials Chemistry
and Engineering, Kyushu University

Jun-ichiro Hayashi

Our Global COE program has an aim of “establishing a new discipline and developing international human resources for environmentally-friendly utilization of carbon resources”, and has a task of showing how carbon resource sciences should/can be built in terms of the carbon cycle, in other words, making proposals for solutions to both problems of environment constraint, which is described with keywords such as global warming and CO₂ emission, and its reverse side, namely, constraint of fossil resources. “Student Forum on Novel Carbon Resource Sciences (NCRS)” was established in 2009 with the goal of making such proposals¹⁾. We have invited experts inside and outside the university over a wide range of areas (science and technology, economy and policy, etc.) that are directly and indirectly related to carbon resource sciences, asked them for lectures and offering of topics of discussion, tried to recognize the current global situation and issues concerning carbon resource utilization through Q&A and pre-focused discussions, and searched for ultimate carbon resources saving in the future. In conjunction with the Forum, we planned and organized domestic and overseas short-term internships, which will be reported elsewhere.

Student Forum as a whole consists of Forum I, II

and III that focus discussion on “Energy Utilization”, “Energy Saving” and “Environment in Asia” respectively. Each forum is organized by advisors (Program Members and Program Collaborators of the COE), young researchers (assistant professors and PDs) and doctoral students who play the most important role in the debates. We have held 12 lectures or debate meetings since August 2009. Each of lectures and meetings is summarised briefly in Table 1.

In Forum I, several lectures and debate meetings have been held, which focused on highly-efficient utilization of energy and resources concerning not only carbon resources but also atomic and renewable energies, stable energy supply, CO₂ emission and so on. Members learned new technologies that are expected to have significant roles in CO₂ emission reduction, such as high-efficiency coal-fired power generation including Integrated Gasification Combined Cycle (IGCC), CO₂ Capture and Storage (CCS), power generation using renewable energy (wind, solar, geothermal, micro hydro power), high-temperature gas reactor for future atomic power generation. Besides, they have also recognized that every Asian country is facing a lot of non-technological, i.e., economical and/or geopolitical problems in its own way in imple-

menting such advanced technologies.

In terms of stable/sustainable energy supply, especially high-quality electricity, members understood that large-scale introduction (even if it were possible at all) of power generation from renewable energy, which inevitably has significant output fluctuation, could cause much load fluctuation and lowered electrical efficiency of thermal power generation, and as a result, make it difficult to attain even reduction of net consumption of fossil resources even if new power operation systems such as smart grids were applied. This possibility was more than a little shocking to those who had simply expected positive effects of renewable energy on reduction of fossils consumption. We are planning to try to draw a proposal that links stable energy supply and highly-efficient conversion of carbon resources on the basis of the result of discussion on storage technology (which was already discussed in Forum II) and possibility and effectiveness of hydrogen and other resources as secondary chemical energy.

The joint debate meeting of Forum I and III focused on Peat Fire in Indonesia which is causing massive CO₂ emission hidden behind that



Table 1 List of Forum

Forum	Date	Theme	Titles and Lecturers	Participants
I&II	2009.8.22	Development of IGCC Technology/ Explanation of CCS	"Development of IGCC (Integrated Coal Gasification Combined Cycle) Technology" Saburo Hara (Central Research Institute of Electric Power Industry) "Explanation of CCS (Carbon dioxide Capture & Sequestration) Technology" Tatsuro Harada (Kyushu Electric Power Company)	57
III	2009.11.30	Tasks and Approaching of Asian Energy Consumption in Low-carbon Society (current status, policy, incentive)	"Energy issues and measures against global warming in China" Jusen Asuka (Prof., Tohoku University) "Measures for Energy Saving and Environment Conservation Taken Overseas by Kyushu electric Power Co., Inc." Takahiko Funakoshi (Kyushu Electric Power Company, Inc.) "Evaluation of saving energy as a measure against global warming" Shunsuke Managi (Associate Prof., Yokohama National University)	41
I&III	2009.12.5	Peat: CO ₂ Emission Source or Carbon Resource?	"Annual Peat Fires in Humid Tropics of West Kalimantan, Indonesia and the Consequences on Peat Carbon Storage, and CO ₂ -e Emission" Gusti Z. Anshari (Centre for Wetlands People and Biodiversity, Tanjungpura University, Indonesia) "Recent Progress in Indonesian Peat Utilization Research" Anggoro Tri Mursito (LIPI: The Indonesian Institute of Sciences, Indonesia)	51
II&III	2009.12.19	System-based Energy Saving: Efficient Energy Utilization Technologies	"Ultimately Efficient Use of Energy over the Edison's Paradigm and the Ford's" Teruhide Hamamatsu (Director General, UXSEP Research Laboratory, Senior Advisor Emeritus for CRIEPI) "Chemical Heat Pump for Waste Heat Utilization in Industrial Field" Yukitaka Kato (Associate Prof., Tokyo Institute of Technology) "The Effect and Potential of Heat Pump Technology for Business and Residential Sector" Takashi Yatabe (Tokyo Electric Power Company)	55
II	2010.1.23	Material-based Energy Saving	"The Role of Chemical Industry for a Sustainable World" Hisao Urata (Mitsubishi Chemical Holdings Corporation) "Automotive Plastics and Rubber Recycle" Norio Sato (Toyota Central R&D Labs., Inc.) "Case study of production efficacy; Point of view from Custom manufacturing industry" Sota Kurita (Lanxess K.K.)	42
I	2010.1.30	Power from Renewable Energy	"What are Solar Cells? How it Works for Clean and Green Society?" Koichi Kakimoto (Prof., Kyushu University) "Development of a Highly Efficient Wind Turbine with Wind-Lens Technology" Yuji Ohya (Prof., Kyushu University)	32
III	2010.2.8	Urban Environment in Asian Mega-cities	"City Ventilation for Better Urban Air Quality and Energy Efficiency" Yuguo Li (Prof., The University of Hong Kong; Presenter: Dr. Lina Yang) "Compact City Planning for Low-Carbon Society" Atsushi Deguchi (Prof., Kyushu University)	28
FY2009 NCRS Forum Discussion	2010.6.19		(1) Energy Best Mix Efficiency in Coal Fired Power Generation, Solar Power Generation, Wind Power Generation (2) Think about CO ₂ CCS, Peat Fire (3) Energy Saving Heat Pump, Growth Strategy for Chemical Industry (4) Asian Environment Environment and Energy Conditions in China, City Planning	49
I&III	2010.7.10	Geothermal Power Generation and Micro Hydraulic Power	"Small Hydropower: its potentials and possibilities" Hisashi Kobayashi (Prof., Ibaraki University) "Volcano and Utilization of Geothermal Energy" Sachio Ehara (Prof., Kyushu University)	36
I&II&III	2010.8.28	Main Issues of Li-ion Battery	"Material Risk and the Strategy in Japan" Kohmei Halada (National Institute for Materials Science) "Global Trends of R&D Projects of Li-ion Battery" Kuniaki Tatsumi (National Institute of Advanced Industrial Science and Technology) "General View of Lithium-Ion Cell Safety" Shinichi Tobishima (Prof., Gunma University)	42
I&II	2010.9.4	Future Technologies of Electric Power Generation and Grid Management	"Digital Grid: Communicative Electrical Grid of the Future" Rikiya Abe (Prof., The University of Tokyo) "Digital Grid: Communicative Electrical Grid of the Future" Hirofumi Ohashi (Japan Atomic Energy Agency)	27
II&III	2010.9.18	Electronic Information Displays and Ecology	"Green Technology in LCD" Jae-Jin Lyu (Samsung Electronics Co., LTD.) "OLED displays: Organic Electronics as Next Generation Green Technology" Tetsuo Tsutsui (Prof., Kyushu University) "Introduction of Electronic Paper Technologies" Reiji Hattori (Prof., Kyushu University)	34

Forum I (Efficient Energy Utilization) Forum II (Energy Saving) Forum III (Asian Environment)

resulting from activities of industrial and civil sectors. Participants learned that it was a sort of human disaster caused by unreasonable land development. Although the debate on "Is peat a resource or an undevelopable carbonaceous component?" heated up, we shared a common understanding that our knowledge of the peat and peat

fire is insufficient as to propose a way that can balance environment conservation and resource development.

Forum II has discussed topics offered from the viewpoints of how to raise availability of electric power and heat derived from fossil resources

(energy-saving systems, devices and materials) and how to make more effective use of carbon resources as chemical feedstock (resources saving). Members came to understanding that large-scale introduction of heat pump, which pumps environmental heat as exergetically low-grade but huge heat of air to electric energy, has a significant potential for CO₂ reduction in combination with carbon resources saving in power generation sector, and also that chemical heat pumps have a great potential in industrial sector. Many students and professors (including myself) seem to have reacknowledged the importance of such new ideas based on very basic thermodynamics and its principles.

Chemical industry has such a complex system that it has become difficult to argue energy and





resources saving, but we learned that nonetheless several innovative attempts and practices for introduction of elemental technologies and systems are in place and becoming clues for new concept formation. "Carbon resources saving" can be discussed more deeply (partly because carbon is fundamental reductant for metal resources, etc) in relation to "element strategy", the topic of which was offered subsequently in Forum II, so we can expect some proposals on sustainable utilization of carbon resources (eg. on the possibility of utilization cycle) to be reached through such discussions.

In addition to the topics mentioned above, the subjects of debate in Forum II involve energy

saving/storage as key technologies in future electric power management and utilization. Topics of lithium-ion batteries, LC display, organic EL and others were offered and tasks toward their improvement and diffusion have already been discussed. Future comprehensive discussion on such technologies for storage and energy-saving devices, preferably ion combination with those for power generation and supply, seems to be essential for the completion of our proposal.

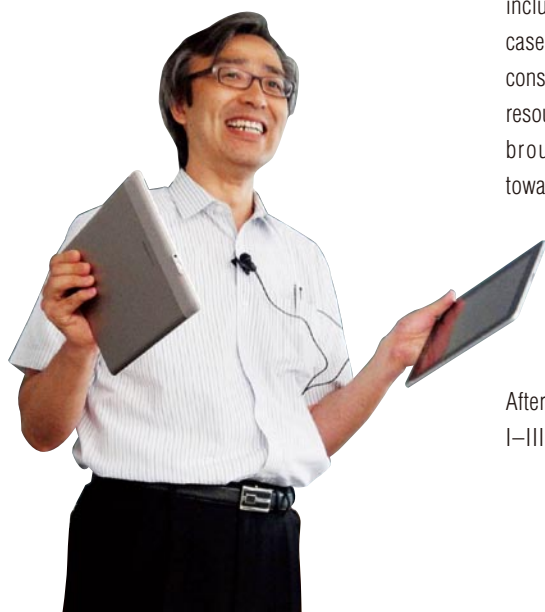
Forum III has tackled the issue of "Environment in Asia", which is not easy to argue for non-experts without broad background knowledge of humanities and sciences. Topics on introduction of technological systems (eg. ECSO) were offered, including topics on solution policy (eg. CDM) for cases in China with large and increasing fossils consumption. The discussion revealed difficulty of resources saving and CO₂ reduction in China, and brought home to us necessity of movement toward concept formation for an extremely heavy challenge inevitable for Novel Carbon Resource Sciences, that is, establishment of a new framework of carbon resource utilization across Asian countries.

After some Joint Forums between I-II, II-III and I-III, all three Forums joined together at the

general discussion meeting for making a midterm summary in June 2010. The organizer offered four topics for discussion: 1. Energy Best Mix (Examples of keyword: high-efficiency technology of coal thermal power generation, renewable energy); 2. Reconsideration of CO₂ related problems and solutions (CCS, peat fire); 3. Energy Saving (heat pumps, growth strategy of chemical industry); 4.Environment in Asia (environmental and energy situation and urban planning in China). Each topic was firstly discussed at each of four sub-sessions, and opinions offered were presented and discussed again at the plenary session.

The session, contributed by about 50 people, became more and more heated up as the discussion proceeded, and with the help of doctoral students, especially foreign ones, it seems to have found a lot of different ideas and viewpoints as well as some points of consensus. In the meeting, the following issues became the points of argument.

- (1)Best or optimum way of utilizing carbon resources that can make world' s economic development and conservation of the carbon cycle system compatible with each other
- (2)Most reasonable ways of carbon resources utilization that can make world' s economic





development and environmental conservation compatible with each other (especially in case of Asia)

- (3) Main roles of developed and developing countries for simultaneous realization of (1) and (2) above.

In one of the three groups, in which I joined the discussion as a moderator, I found very interesting points of consensus and common concern. The summary is as follows.

- Higher-efficient utilization of carbon resources is vital for Asian countries even though we face either or both of global warming and shortage (or depletion in the future?) of carbon resources. It must be, however, associated with the economic growth.
- CO₂/GDP may be useful as an index reference to compatibility of economic growth and realization of low carbon society, and it may be suitable for Japan. It is, however, not reasonable to apply such a Japan model directly to other Asian countries. How can we break the link between growth of GDP and increase of CO₂ emission in a suitable way for each country or each region?
- At least some of Asian countries reserve a plenty of carbon resources and then the capacity of exporting them. Can we establish a new chemical industry in such countries for

creating high added value of carbon resources, especially of low rank coal (as it is called so far) and biomass resources, or ultra energy saving? What is the role of Japan for realizing that?

- We should orient toward a pan-Asian community. Isn't there any possibility of creating a community which establishes an international division of labor concerning resources, energy, materials, chemical products and related industries? What role can or should be taken by each country?

In the joint session, so many comments were offered that I do not have enough space to make a summary here, but I believe that an orientation was found toward a pan-Asian community again in the comments concerning environmental and chemical industries. Though we could not offer any clear answers to the topic (3) noted above in the session, it is hopefully possible to find one or more lasting roles (or functions) of each country in a pan-Asian community taking social and economic system, culture and other aspects of each region well into consideration. On the basis of such discussion, it is expected to make a proposal to envision a basic science and technology for innovative principles/ways of carbon resources utilization, energy saving and environmental preservation. In my personal view

(although it may be too exaggerated), Novel Carbon Resource Sciences can be a transnational fusion of social science, natural science and engineering, as one example of "Fusion of science and technology", which has long been sought for.

We have reviewed the first year of NCRS Forum. Although we still have a lot of things to think about, continuous participation in the Forum may already have encouraged the students to contemplate their own specialized advanced research as situated within the whole system, by experiencing Novel Carbon Resource Sciences as a comprehensive (in other words, so wide-ranging and still vague) field even in an elementary way. Or some students might have realized that not only knowledge of specific fields, but also more cultivation (including knowledge of basic sciences) was needed for them as researchers. If so, it can be said that the NCRS Forum has already been assumed one of its important roles.

Cited Reference

- 1) Hideo Nagashima, "Start on NCRS Forum", Kyushu University Global COE Program "Novel Carbon Resource Sciences" Newsletter, Vol. 2 (2010).

(Kuwait — November 1, 2010) - Kuwait Institute for Scientific Research (KISR) organized a ceremony for the signing of an agreement with Japan Cooperation Center, Petroleum (JCCP) regarding a joint research project entitled "Research on Upgrading Technology of Kuwait Heavy Crudes".

Hideo Nagashima

Professor, Program Leader
Institute for Materials Chemistry and Engineering, Kyushu University

KISR collaboration with JCCP started in 1993 and continuously strengthened over the past years. Since 1993, the fruitful collaboration between KISR and JCCP resulted in more than 21 research projects and more than 11 symposiums. The present project is unique since the technical collaboration between JCCP and KISR is extended to universities, namely, Kyushu University, in addition to refining companies in Japan.

The joint project between KISR and JCCP will be technically supported by Kyushu University and JX Nippon Research Institute Ltd. The project aims to study the characteristics and behavior of typical Kuwait Heavy Crudes which will be having substantial attention on the coming years for Kuwait Refining Industry, namely, gas oil (GO)

and atmospheric residue (AR) from Ratawi-Burgan, Eocene and Lower Fars crudes. The options on processability of these fractions to produce high quality of petroleum products with international specifications based on the findings will be approached. Data specific to the Kuwaiti feedstocks is either scarce or not available.

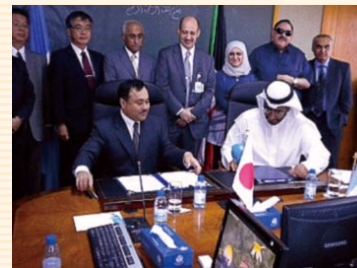
The joint project will lead to establish the scientific and technical data for these crudes and comparison with Kuwait Export Crude (KEC) which being used and practiced at Kuwait refineries for decades. The information obtained will be useful for future refining industry at KNPC.

Japanese side:

1. Mr. Yasuyoshi KOMIZO, Ambassador of Japanese Embassy in Kuwait
2. Mr. Takanori YAMASHITA, First Secretary of Japanese Embassy in Kuwait
3. Mr. Morihiro YOSHIDA, Managing Director, JCCP
4. Mr. Kenji NITA, General Manager, Riyadh Office, JCCP
5. Mr. Nobuyuki SUYAMA, Manager, JCCP
6. Prof. Hideo NAGASHIMA, Vice President, Kyushu University
7. Prof. Isao MOCHIDA, Professor, Kyushu University
8. Mr. Masamitsu TAKANO, Manager, JX Nippon Research Institute, Ltd.
9. Dr. Hiderhiro Higashi JCCP/KISR

Kuwait side:

10. Dr. Naji M. Al-Mutairi, Director General
11. Dr. Mohammed Salman, DDG/Research
12. Dr. Nader Al-Awadhi, DDG/Information
13. Ms. Sahera Al-Dousari, DDG/A&F
14. Dr. Abdulhameed Al-Hashem, Director/PRSC
15. Dr. Meena Marafi, DM/PRD
16. Dr. Mohammed Al-Ramadhan, KPC
17. Mr. Ahmad Al-Jimaz, DMD/Shuaiba Refinery
18. Mr. Mohammad Ghazi Al-Mutairi, DMD/MAB Refinery
19. Ms. Badriya Farhad, KOC
20. Mr. Khalid Al-Mushaileh, KNPC
21. Dr. Suad Al-Radwan, MAA, KNPC
22. Dr. Adel Al-Abbasi, KOC
23. Mr. M. Al-Homoud, OMPM/KISR



Signing Ceremony



Speech by Prof. Hideo Nagashima, the Leader of our COE



Ceremony reported on local newspapers in Kuwait

SYMPOSIUM & WORKSHOP

SYMPOSIUM

The 5th International Symposium on Novel Carbon Resource Sciences

Date: April 21-23, 2010

Venue: Curtin University of Technology, Perth, Australia

The 20th Banyu Fukuoka Symposium — New Paradigm of Creation through Current Synthetic Organic Chemistry —

Date: May 22, 2010

Venue: Centennial Hall Kyushu University School of Medicine

The 6th International Symposium on Novel Carbon Resource Sciences

— Aiming toward Low-Carbon Society —

Date: November 12-13, 2010

Venue: C-CUBE 1st floor Chikushi Hall at Chikushi campus, Kyushu University

Cross Straits Symposium on Materials, Energy and Environmental Sciences¹²

Date: November 17-18, 2010

Venue: Pohang University of Science and Technology, Gyungbuk, Korea

GCOE NCRS Public Lecture — Let's think about greenhouse gas CO₂ reduction —

Date: November 27, 2010

Venue: University Assembly Hall, Fukuoka Women's University

The 3rd International Symposium on Human Life and Environment

— Health condition considering residence and regional environment —

Date: December 3, 2010

Venue: Kitakyushu Science and Research Park

The 23rd International Symposium on Chemical Engineering

Date: December 4, 2010

Venue: Kyushu Sangyo University Bldg. No.1

The Second International Symposium on Gasification and Its Application (iSGA 2010)

Date: December 5-8, 2010

Venue: THE LUIGANS, Fukuoka

International Symposium on Earth Science and Technology 2010

Date: December 7-8, 2010

Venue: INAMORI International Hall, Ito campus, Kyushu University

WORKSHOP

3rd G-COE International Workshop on Energy and Environment in Chemical Engineering

Date: May 31, 2010

Venue: Research Center for Steel at Ito Campus, Kyushu University

International Workshop on Process Intensification 2010

Date: December 2-3, 2010

Venue: INAMORI International Hall, Ito campus, Kyushu University

LECTURE & SEMINAR

NCRS G-COE Special Seminar

Date: May 21, 2010

Venue: Central Bldg. of IMCE at Chikushi Campus, Kyushu University

IAS Seminar: Nobel Prize in Chemistry K.BARRY SHARPLESS, PhD Special Lecture

Date: May 21, 2010

Venue: INAMORI Center Building, Ito Campus, Kyushu University

IMCE / GCOE NCRS Lecture

Date: June 2, 2010

Venue: IGSES Bldg., Chikushi campus, Kyushu University

JLCS Lecture & Discussion

Date: September 5-8, 2010

Venue: Centennial Hall School of Medicine

Co-sponsored Seminar

Lecture organized by Research and Education Center of Carbon Resources, Kyushu University

Date: May 31, 2010

Venue: C-CUBE 1st floor Chikushi Hall at Chikushi campus, Kyushu University

The 49th Industrial physical chemistry workshop — Electric system and device development to structure Low energy society —

Date: October 22, 2010

Venue: INAMORI Foundation Center, Ito Campus, Kyushu University

The 145th KASTEC Seminar

Date: December 3, 2010

Venue: Art, Science and Technology Center for Cooperative Research, Chikushi Campus, Kyushu University

Lecture organized by Research and Education Center of Carbon Resources, Kyushu University

Date: December 10, 2010

Venue: C-CUBE 301 at Chikushi campus, Kyushu University

Research Performance 2010

Awards & Articles

●Award

2 research papers by Prof. Masaki Minemoto et al got an award for excellence 2009 in KAGAKU KOGAKU RONBUNSHU. (2009/03)

Yosuke Matsukuma, Takafumi Inoue, Yukihiisa Ijuin, Gen Inoue and Masaki Minemoto
"Uniformization of Flow through a Honeycomb Structure by the Lattice Boltzmann Method"

Hideki Itou, Shigeru Tsurumaki, Takuya Moriga, Akihiko Yamada, Shigeru Nojima, Gen Inoue, Yosuke Matsukuma and Masaki Minemoto
"Prevention of Degradation of a Polymer Electrolyte Fuel Cell"

●Award

Japan Society of Refrigerating and Air Conditioning Engineers, Encouragement Prize 2009 (2010/05)

Shigeru Koyama, XUE Jun, Ken Kuwahara
"Performance Prediction Method of CO₂ Heat Pump Cycle for Air-conditioning"

●Award

The 19th JEC Environmental Chemistry Technology Prize (2010/06)

Tetsuya Satsubashi, Chisato Tsukahara, Ayako Ureshino, Tomoharu Nakao, Keigo Baba, Yoshinori Fukunaga and Norio Miura
"Search for Optimum Adsorbent of Polychlorinated Biphenyl for Online Solid-phase Extraction"

●Award

Asian Core Program Lectureship Award (Taiwan) (2010/11)

Hideo Nagashima
"Catalysis in Siloxane Gels"

●Award

Asian Core Program Lectureship Award (Singapore) (2010/11)

Katsuhiko Tomooka
"Asymmetric Synthesis of Chiral Silanol and Its Transformation"

●Award

The Society of Synthetic Organic Chemistry Japan 2010, Excellent Thesis Award (2010/12)

Kazunobu Igawa, Naoto Kokan, and Katsuhiko Tomooka
"Asymmetric Synthesis of Chiral Silacarboxylic Acids and Their Ester Derivatives"

●Award

The 9th International Symposium on Advances in Electrochemical Science and Technology (ISAEST-9), The Best Paper Award (2010/12)

K. Chihara, T. Doi, S. Yatomi, S. Okada, J. Yamaki
"Electrochemical Properties of Monodisperse Nano-size LiMnPO₄ and LiFePO₄ Prepared by Liquid Phase Synthesis Method"

●Award

The 47th Joint Kyushu Meeting of Branches Related to Chemistries, Young Scientists Award (2010/07)

Takahiro Ueno
"Device characteristics of an organic memory of gold nanoparticle/hyper-branched polymer composite film"

●Award

The 47th Joint Kyushu Meeting of Branches Related to Chemistries, Young Scientists Award (physical chemistry) (2010/07)

Akihiro Tou
"Catalytic Property for NO-CO Reaction of Pd-LaMnO₃ Catalyst Supported in and out of Pore of Alumina"

●Award

Best Presentation Award TOCAT6/APCAT5 Youth Session (2010/07)

Kana Kimura
"Preparation of Highly Dispersed Platinum Catalysts on TiO₂ by Using Polymer-protected Nanoparticles"

●Award

Best Poster Presentation Award at the 5th Pacific-Rim Conference on Rheology (PRCR-5) (2010/08)

Hu Hao
"Viscoelasticity of Pullulan in Ionic Liquid Bmim Cl"

●Award

Youth Poster prize in MMIJ Annual Meeting 2010 (2010/09)

Sayo Moriyama
"Removal of Borate with Magnesium Oxides Prepared at Different Temperatures"

●Award

Best Poster Presentation Award in the 24th Diamond Symposium (2010/11)

Shinya Ohmagari
"Ultraviolet Light Detection of p-type Ultrananocrystalline Diamond-Hydrogenated Amorphous Carbon Films/n-type Si Heterojunctions"

●Award

Incentive Award of The Japan Institute of Energy (2010/11)

Tatsuya Wakeyama
"Analysis of Renewable Energy Resource Potential with Quantitative Evaluation in Kyushu Area, Japan"

●Award

Best Poster Presentation Award at the 2nd Semiconductor Materials and Devices Forum (2010/12)

Shinya Ohmagari
"Application of Ultrananocrystalline Diamond/hydrogenated Amorphous Carbon Composite Films to Optical Electrical Devices"

●Report

Professor Norio Miura, whose research paper was cited many times, was selected a world 'remarkable' out of 277 researchers as a much contributor to the field of engineering by ISIHighlyCited.com. (2010/11)

Norio Miura
ISIHighlyCited.com (<http://isihighlycited.com>)



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