### **HU-ACE NEWS LETTER**

**Advanced Core for Energetics**, Hiroshima University



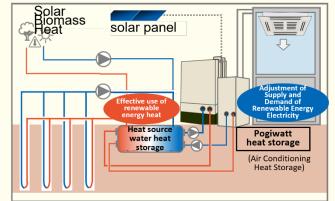
### Activities of the Core

June. 11, 2024	The 14th Hiroshima University Biomass Premium Evening Seminar (co-organized by HU-ACE)
June. 15, 2024	The 1st Higashihiroshima-Ene/Eco Seminar (co-organized by HU-ACE)
June. 19, 2024	The 92nd HU-ACE Steering Committee Meeting
June. 22, 2024	The 2nd Higashihiroshima-Ene/Eco Seminar (co-organized by HU-ACE)

### Geothermal energy seminars are held regularly

The 7th Geothermal Energy Seminar was held on May 22. The seminar, hosted by HU-ACE, has been conducted online about once every months since 2022. Each seminar is attended by approx. 60 participants from various fields both inside and outside HU, and has been successful with active discussions as well as valuable lectures. The lecturers, who are researchers or engineers with a great deal of practical experiences in ground source utilization in actual buildings, provide us with insightful discoveries and suggestions that will lead to the future spread of ground source utilization. In particular, unlike general conferences, the seminar offers a valuable opportunity for audiences to

hear the lecturers' design philosophy, such as how to reasonably apply ground source systems, which require higher initial costs than conventional air conditioning systems. HU-ACE will take action through ground source utilization to achieve the HU Action Plan aimed at realizing a carbon neutral society. We look forward to your continued participation in our seminars.



#### Fig. Conceptual diagram of double heat storage air conditioning system

### **Related Events**

The 8th International Symposium on Fuels and Energy (ISFE2024) is scheduled on July 1-2, 2024. June 27 is the deadline for standard registration. Details can be found here. <u>https://symposium2024.isfe.hiroshima-u.ac.jp/</u>

We have constructed a roadmap for the development of energy utilization technologies leading up to 2050 and an integration scenario called the "Hiroshima Scenario". Please feel free to share your thoughts with us. <u>https://hu-ace.hiroshima-u.ac.jp/wp/wp-content/uploads/2022/10/220921-brochure.pdf</u>



### research consultation and joint research are welcome.

Issued by Advanced Core for Energetics, Hiroshima University HU-ACE Secretariat, URA Division, Office of Research and Academia-Government-Community Collaboration, Hiroshima University 1-3-2 Kagamiyama, Higashi-Hiroshima, 739-8511 Japan E-mail: hu-ace-info@ml.hiroshima-u.ac.jp, tel:+81-82-424-4425, URL: https://hu-ace.hiroshima-u.ac.jp/en/ alcohol fuels

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## **Research** Topics

# **Combustion chemistry of carbon-neutral**

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Research fields: Combustion engineering/chemistry, Chemical kinetics Keywords: Detailed kinetics of combustion, Engine combustion and fuel

### Abstract

### Background

Transition to renewable energy is inevitable for mitigation of climate change and global warming. For this purpose, some automobiles will be replaced by electric cars while high energy-density liquid fuels such as gasoline and diesel oils are going to be produced from carbon-neutral energy sources. These liquid fuels should not need to mimic those derived from fossil oil. If fuels more appropriate for automotive engines can be provided, the engine performance will increase and result in depletion of carbon dioxide emission. So, what are the appropriate fuels? The goal of our research is to answer this question.

### **Methods**

To answer the question, researches are undertaken as joint projects among researchers of automotive companies, oil companies, and universities. In these, my role is, by elucidation of reaction mechanisms of combustion, to answer why this fuel is good. Combustion is chemical reaction consisting of a huge number of elementary processes. The mechanisms are constructed from the accumulated experimental and theoretical knowledge supplemented by quantum chemical or other Then, by numerically solving the system of ODEs of calculations. elementary reactions, combustion phenomena are reproduced and analyzed. Here examples of such numerical calculations are shown.

### **Results**

Figure 1 shows non-additive response of ignition delay time when ethanol was mixed with hydrocarbon fuels, and at 877 K, maximum anti-knock property can be found. This phenomenon is called octane hyperboost and can be observed in prenol or ethanol mixture with hydrocarbon fuels. This phenomenon cannot be properly reproduced by the existing chemical kinetic mechanisms. We reinvestigated the relevant rate constants by quantum chemistry. The results showed that, as shown in Fig. 2, the treatment of hydrogen-bonding and non-hydrogen-bonded transition states is key to this problem and that the previous rate constants were underestimated. These results improved the reproduction of the octane hyper-boost phenomenon, and will contribute to the future development of carbon-neutral alcohol fuels.

### References

1. (a) E. Monroe et al., Fuel, 239, 1143 (2019). (b) Ueda et al, Shock Wave Symposium, Japan 1A3-3 (2022). 2. Oppata et al., 61st Symposium (Japanese) on Combustion, C314 (2024).

ethanol volume fraction Fig. 1 Octane hyper-boost.

0.5

1.0

