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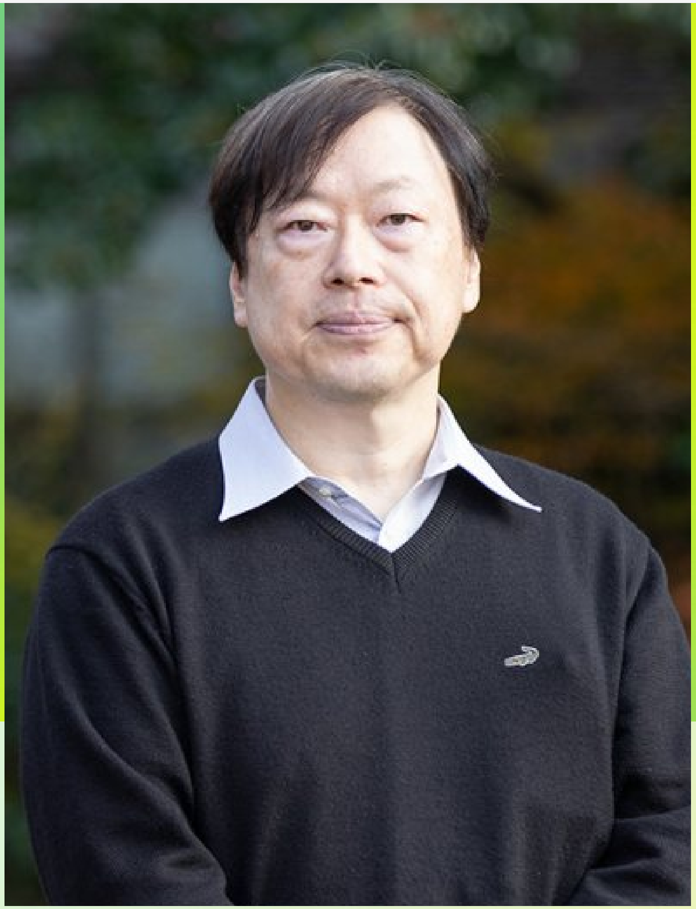
Challenging Decarbonization: Next-Generation Ammonia Fuel

Contributing to Burner Design through Ammonia Combustion Simulation



Because ammonia does not emit carbon dioxide when burned, attention is turning to its potential as a fuel for achieving carbon neutrality by 2050. However, ammonia is generally a difficult substance to burn, and forcibly combusting it may result in the emission of harmful NOx exceeding environmental standards. To address these challenges through combustion methods, Dr. Yukihiko Okumura from Kagawa University is advancing research through a dual approach of experimentation and simulation. Obtaining insights unique to simulations that cannot be gained through experiments alone, Dr. Okumura arrived at a “tornado burner” that safely and efficiently burns pure ammonia.

Yukihiko Okumura
Professor, Faculty of Engineering and Design, Kagawa University

Ammonia Fuel: More Cost-Effective and Energy-Efficient than Hydrogen

With an eye on achieving carbon neutrality by 2050, a movement is arising to realize a hydrogen society. Therefore, a method has been developed in which hydrogen (H_2) is converted into ammonia (NH_3) and transported from overseas, after which the hydrogen is extracted from the ammonia and used. This is done to transport hydrogen, which liquefies at minus 253°C, in a cost-effective and energy-efficient manner. However, Dr. Okumura, explaining the motivation for ammonia burner research, says, “Rather than extracting hydrogen from ammonia and using it as hydrogen fuel, burning ammonia itself allows us to obtain high calories without energy loss. Using additional energy for extracting the hydrogen is also unnecessary.”

However, ammonia is a fire-resistant substance that does not easily ignite even when exposed to flame. Additionally, forcibly burning it releases harmful nitrogen oxides (NOx). National environmental standards stipulate that “NOx emissions should be 150ppm or less for boilers and 600ppm or less for gas engines.” That is why, in 2017, Dr. Okumura began researching how to efficiently combust ammonia with minimal NOx emissions. Three years later, the Japanese government selected Hydrogen/Fuel Ammonia Industries as one of 14 fields in its Green Growth Strategy*1 in December 2020. Reflecting on the time he started studying ammonia combustion, Dr. Okumura says, “Finding a way to use inherently difficult-to-burn ammonia as fuel was a challenge itself. Little was known about ammonia combustion at that time.”

Having conducted combustion research on various substances since his student days, Dr. Okumura believed that understanding the combustion mechanism and flame structure of ammonia was crucial for developing an ammonia burner. Therefore, he decided to pursue combustion research using both experimentation and simulation.

Simulation of Ammonia Combustion

To burn ammonia, a mixed combustion method is commonly used that involves co-burning it with methane (CH_4), the main component of natural

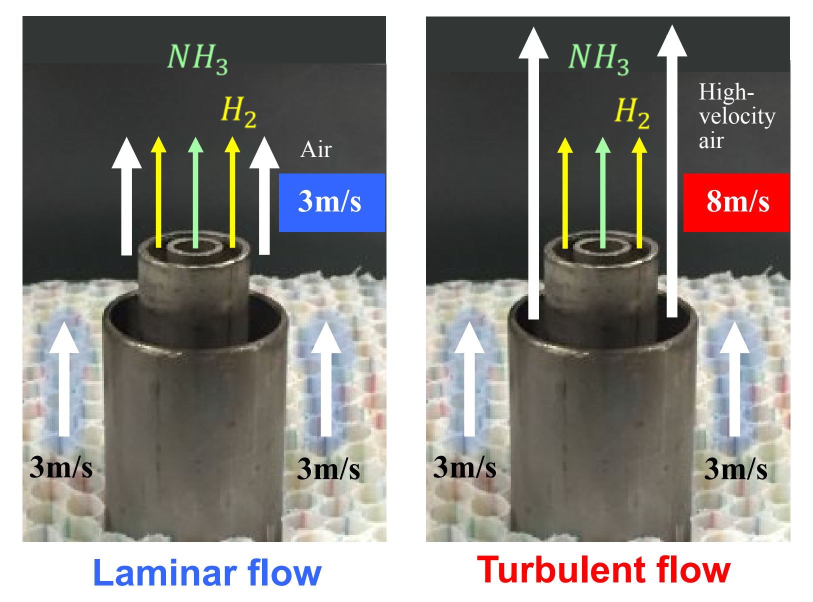
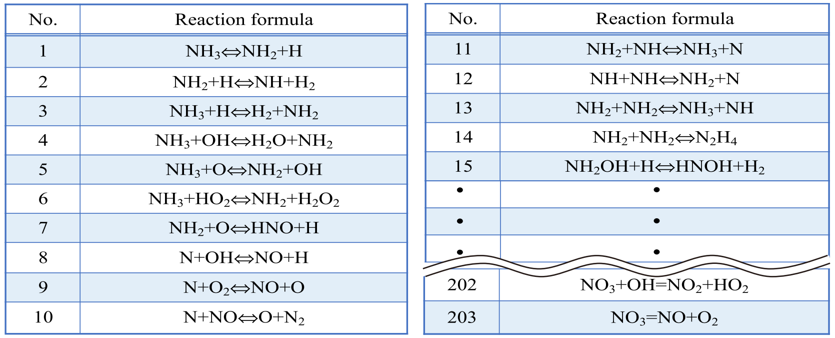


Fig.1 : Ammonia burner used in the research

The space between rims blows out ammonia, hydrogen and air. In the right diagram, turbulence is created by high-speed air (8m/s) flowing faster than ammonia and hydrogen. Generally, turbulent flow results in higher combustion efficiency per unit volume than laminar flow. To streamline the flow around the rim, students in the Okumura Laboratory laid cut straws and directed air at 3m/s. As a result, the calculation of the surrounding airflow was simplified.

gas. However, burning methane produces CO_2 emissions. So Dr. Okumura initiated research on a burner with hydrogen flame stabilizer to assist in the combustion of ammonia using hydrogen gas (Fig. 1). He designed and fabricated the burner so that it could create both laminar flows, in which the flame calmly rises, and turbulent flows, where the fuel is forcibly mixed with high-velocity air and becomes turbulent flame, by adjusting the amount of air sent along with the combustion gas. This allowed him to conduct experiments and simulations under the same conditions.

In experimental studies, temperature was measured at various locations in the flame. Gas measurements were also taken to determine the amounts of major chemical species (H_2, O_2, N_2, NH_3, NOx, H_2O) at those locations. Meanwhile, simulation studies utilized fluid dynamics software called “Advance/frontflow/red” to calculate in detail the distribution and reactions of all chemical species including radical species within the flame, determining how temperature changes with the progression of reactions.



No.	Reaction formula
1	$NH_3 \Leftrightarrow NH_2+H$
2	$NH_2+H \Leftrightarrow NH+H_2$
3	$NH_3+H \Leftrightarrow H_2+NH_2$
4	$NH_3+OH \Leftrightarrow H_2O+NH_2$
5	$NH_3+O \Leftrightarrow NH_2+OH$
6	$NH_3+HO_2 \Leftrightarrow NH_2+H_2O_2$
7	$NH_2+O \Leftrightarrow HNO+H$
8	$N+OH \Leftrightarrow NO+H$
9	$N+O_2 \Leftrightarrow NO+O$
10	$N+NO \Leftrightarrow O+N_2$

No.	Reaction formula
11	$NH_2+NH \Leftrightarrow NH_3+N$
12	$NH+NH \Leftrightarrow NH_2+N$
13	$NH_2+NH_2 \Leftrightarrow NH_3+NH$
14	$NH_2+NH_2 \Leftrightarrow N_2H_4$
15	$NH_2OH+H \Leftrightarrow HNOH+H_2$
•	•
•	•
•	•
202	$NO_3+OH=NO_2+HO_2$
203	$NO_3=NO+O_2$

Fig. 2 : Example of elementary reaction equations for ammonia combustion

The study utilized CRECK’s reaction mechanism (31 chemical species, 203 reaction equations).

The chemical reaction for ammonia combustion can be expressed as $4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$, which is an equation summarizing all the reactions. In fact, within the flame, highly reactive and unstable radicals are produced, changing into other chemical species. There are 31 related chemical species and 203 reaction equations (Fig. 2). Considering all of them is crucial for understanding the details of combustion. Furthermore, the reactions with hydrogen and the surrounding air and flow fields also add complexity to the overall flame picture.

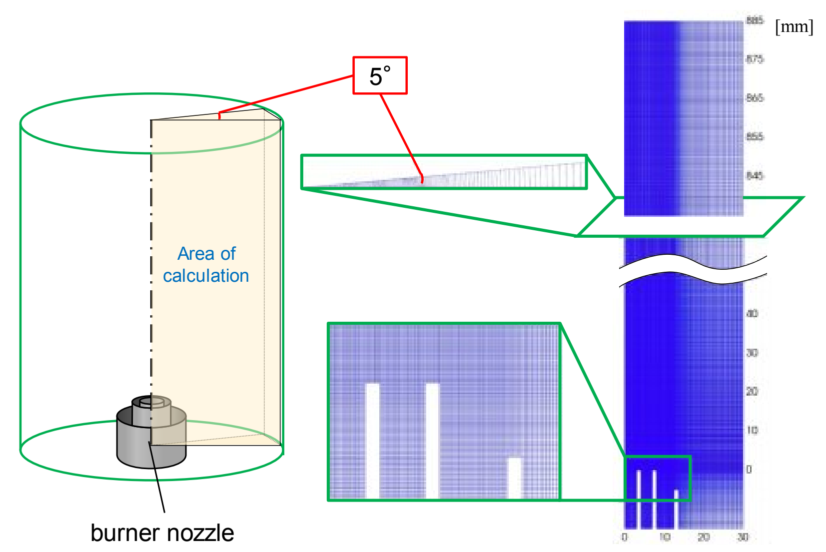


Fig. 3 : Simulation of a laboratory-scale ammonia burner

The area near the gas outlet (rim) employs a fine mesh with 0.1mm squares, while the part away from the rim is coarsely divided to reduce computational load. Assuming axial symmetry, the calculation range covers only 5 degrees rather than the entire circumference.

Fig. 3 - Fig. 6: Reprinted from the Journal of the Combustion Society of Japan, Vol.64 No.208 (2022) 168-176, “Flame Structure and Reaction Analysis for Ammonia Turbulent Burner with Hydrogen Flame Stabilizer,” Okumura, Y., et al., with permission from the Combustion Society of Japan.

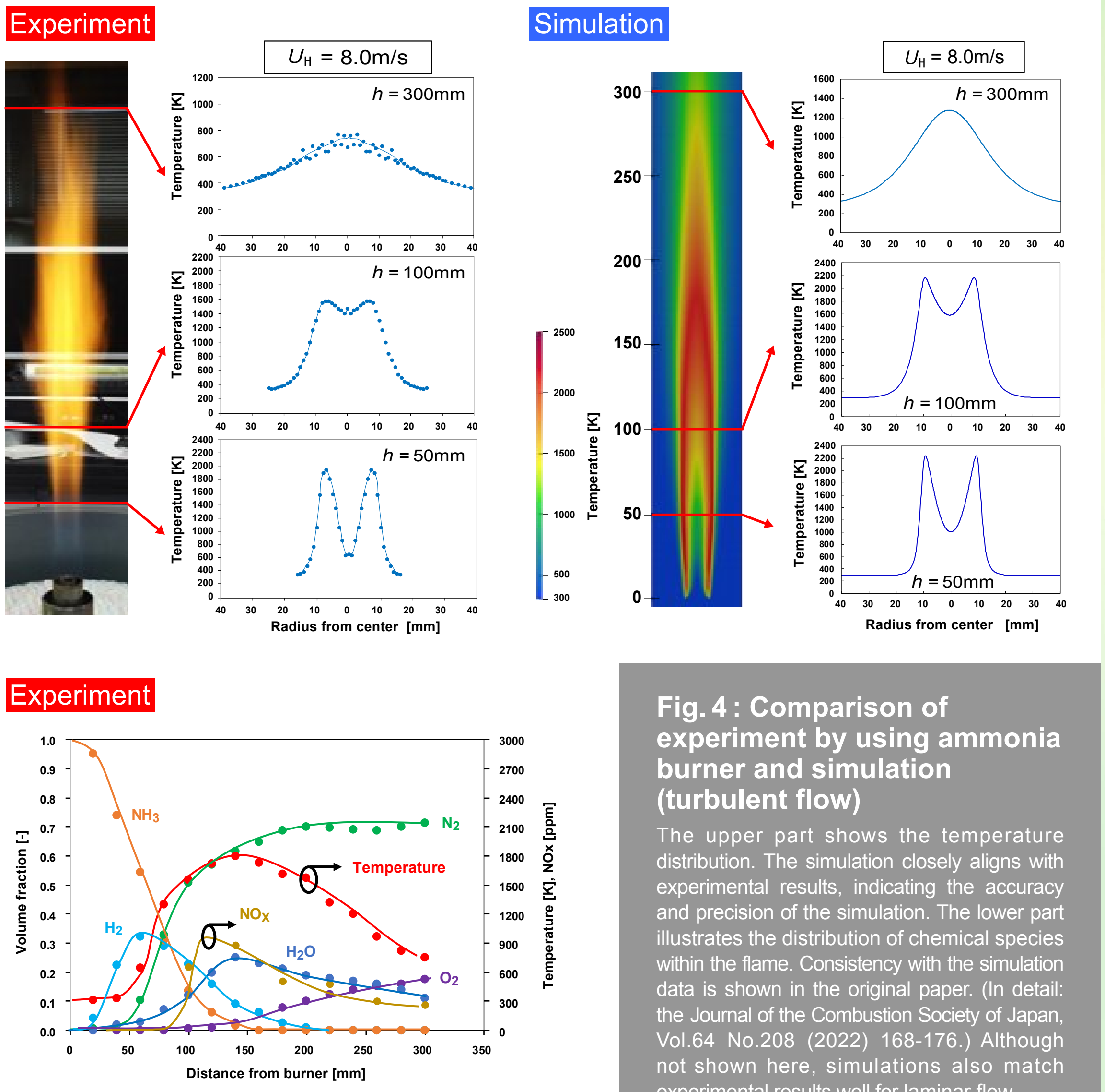


Fig. 4 : Comparison of experiment by using ammonia burner and simulation (turbulent flow)

The upper part shows the temperature distribution. The simulation closely aligns with experimental results, indicating the accuracy and precision of the simulation. The lower part illustrates the distribution of chemical species within the flame. Consistency with the simulation data is shown in the original paper. (In detail: the Journal of the Combustion Society of Japan, Vol.64 No.208 (2022) 168-176.) Although not shown here, simulations also match experimental results well for laminar flow.

“We divided the space occupied by the flame and surrounding air into a grid, solving a governing equations in reactive flow that included mass conservation, energy conservation, and momentum conservation, as well as the state equation of gases and the equation of mass conservation for chemical species (element conservation). Except for the equation of mass conservation for chemical species, this is the same as the atmospheric simulations used for weather forecasting. However, as soon as chemical reactions (elementary reaction groups) are included in the calculations, the computational load becomes enormous,” Dr. Okumura says.

To reduce computational load, Dr. Okumura initially targeted laboratory-scale burners. He explored options to coarsen the grid while maintaining calculation accuracy, assuming axial symmetry and time-averaging turbulence (Fig. 3). For later turbulent calculations for the tornado ammonia burner and large burners, he transitioned to “Fugaku”-class computational resources capable of handling large-scale calculations (360° range and large spatial dimensions).

“At the beginning of the research, I had 69 elementary reaction equations for ammonia combustion. However, calculations at that time, which used a scheme developed based on hydrocarbons, did not agree with the experimental results at all. Concurrently with my research, the elucidation of elementary reactions for ammonia combustion progressed, and the number of reactions related to ammonia increased. It was only when we included 203 elementary reaction equations that we finally obtained calculation results close to experimental results (Fig. 4). Performing calculations with 203 elementary reaction equations was made possible by the computational power of HPCI," Dr. Okumura says.

Simulation Is the Only Way to Understand the Mechanism of Ammonia Combustion in Detail

Dr. Okumura explains the simulation study strengths as follows. "There are limitations to the quantities that can be measured experimentally. Especially, it is almost impossible to determine the spatial distribution of essential radicals for combustion, such as H radicals, O radicals, and NH radicals. In contrast to that, simulation allows us to clarify reactions occurring at every location within the flame." Simulation results have revealed that OH radicals and H radicals move and mix due to turbulence, and that radicals and heat derived from hydrogen fuel particularly promote and sustain the combustion reaction of ammonia (Fig. 5).

Furthermore, Dr. Okumura believes that simulations could differentiate whether a nitrogen in a specific

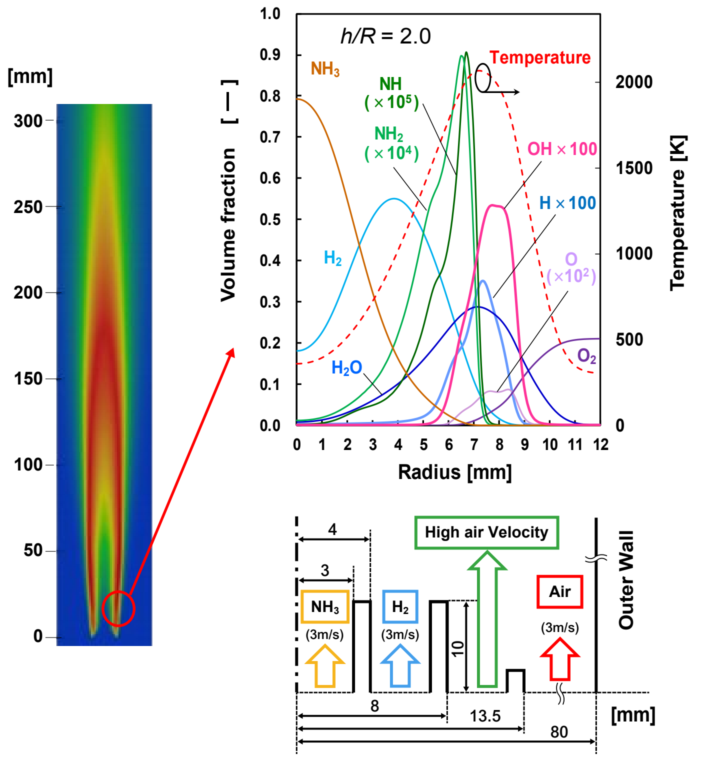


Fig. 5 : Radical concentrations in a turbulent burner with hydrogen flame stabilizer analyzed using the supercomputer "Fugaku"

At left is the temperature distribution of the flame. The upper-right graph shows the temperature and chemical species amounts at the red circle position (flame height of 14mm), and the lower-right indicates the locations where various gases are jetted. Looking at the upper-right graph, the highest temperature is observed in the region of $7<r<9$ [mm] (where air is mixed), and OH radicals (pink line) and H radicals (blue line) that promote combustion reactions are generated more abundantly due to the combustion of supplementary hydrogen. In addition, the heat generated by burning hydrogen is transferred to the ammonia injection part, supplying energy to maintain the combustion chemical reactions of ammonia. The essential OH radicals and H radicals for combustion are diffused through turbulence and forcibly mixed in the region of $5<r<8$ [mm], contributing to the stable maintenance of combustion.

NOx molecule formed from the air or the ammonia. He calculated the combustion process with distinguishing nitrogen atoms derived from ammonia and nitrogen molecules in the air, revealing that the majority of NOx emitted from the top of the flame into the atmosphere is derived from ammonia, with air-derived NOx existing only at the bottom of the flame and overwhelmingly minimal (Fig. 6 (1)).

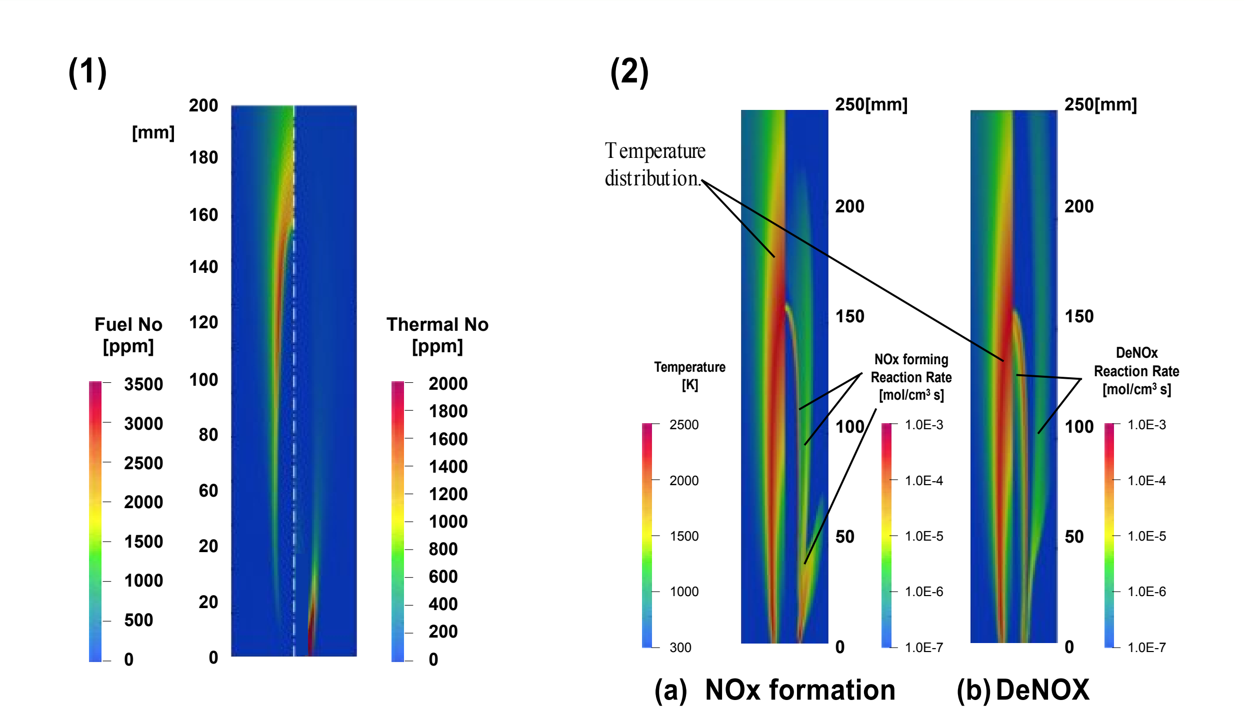


Fig. 6 : Mechanism of NOx formation

(1) The left half shows the distribution of NOx derived from ammonia (Fuel NO). The right half shows the distribution of NOx derived from nitrogen molecules in the air (Thermal NO).
(2) Reaction rates of NOx formation (a) and NOx reduction (b). NOx rapidly disappears in the region near its intense creation at a rate comparable to the formation rate.

Reflecting on the simulation, Dr. Okumura notes, “NOx did not reach extremely high levels.” The reason became apparent also through the simulation. Nitrogen atoms are oxidized to form NOx molecules, and they turn into N_2 molecules, when reduced. Analyzing where and how much of this oxidation-reduction reaction occurs, it was found that NOx is primarily generated in the slightly inner region of the high-temperature zone of the flame where fuel is abundant, and at almost the same location, reduction reactions also effectively eliminate NOx (Fig. 6 (2)). “It became clear that the contribution of the reduction reaction is significantly large, although the reaction rate of NOx generation is higher than that of NOx reduction. This knowledge, obtained through simulation, explains why there was no extreme increase in NOx concentration. It underscores the significance of simulation research in providing insights into reactions and flame structure,” Dr. Okumura says.

Promoting Ammonia Burners in Industrial Settings and Achieving Carbon Neutrality by 2050

In the industrial sector, initiatives are already underway to replace burners, used in processes such as breaking down naphtha obtained from petroleum refining for plastic production and pottery kiln firing, with ammonia burners. Dr. Okumura aims to popularize ammonia burners that can be used in industrial settings. To achieve industrial applications, it is crucial to realize ammonia combustion that meets environmental standards at low cost. Consequently, Dr. Okumura has also initiated research on an “ammonia dedicated burner,” which can combust ammonia without using expensive hydrogen.

Recognizing the importance of continuously generating active radicals to sustain ammonia combustion, Dr. Okumura devised the tornado burner. This burner releases a pre-mixed gas of ammonia and air from the bottom, and additionally injects it from the side of the cylinder, swirling the flame.

In this research, a combination of simulations using Oakbridge-CX at the University of Tokyo and experiments were employed to investigate the ratios of ammonia to air (equivalent ratio), flow velocities, and other factors for the main jet and swirling jets (Fig. 7). Successful results were achieved, showcasing the conditions for ammonia-dedicated combustion. The NOx emission level was also lowered, nearly reaching environmental standards due to the two-stage combustion method and tornado effect. Furthermore, technology has been developed to reduce unburned ammonia below environmental standards even with a large flow of ammonia injection.

Dr. Okumura emphasized the strength of experimental research in being able to cross-check simulation results, stating that experimental results are undeniable facts even if the combustion process is unstable or does not fit the theory. He highlighted the synergy between simulation and experimental research, describing them as the “two wheels” of a vehicle. Striving to introduce ammonia burners for industrial use promptly, Dr. Okumura is accelerating the research, leveraging both aspects. He expressed his aspirations, saying “My combustion technology (ammonia dedicated burner) has come very close to completion and I hope my technology will contribute to achieving carbon neutrality by 2050.”

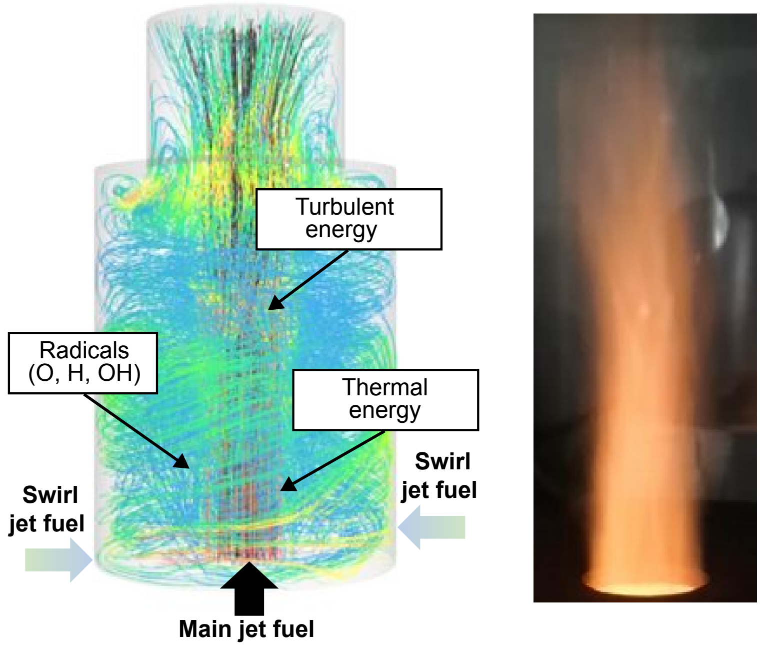


Fig. 7 : Simulation and actual combustion of tornado ammonia dedicated burner

The tornado burner enables combustion of the flame-retardant ammonia without the need for hydrogen. Simulation results revealed that the main jet and swirling jet mutually supply thermal energy, turbulent energy, and radicals. Numerous improvements have been made to the presented burner, bringing it closer to meeting the exhaust characteristics that comply with environmental standards.

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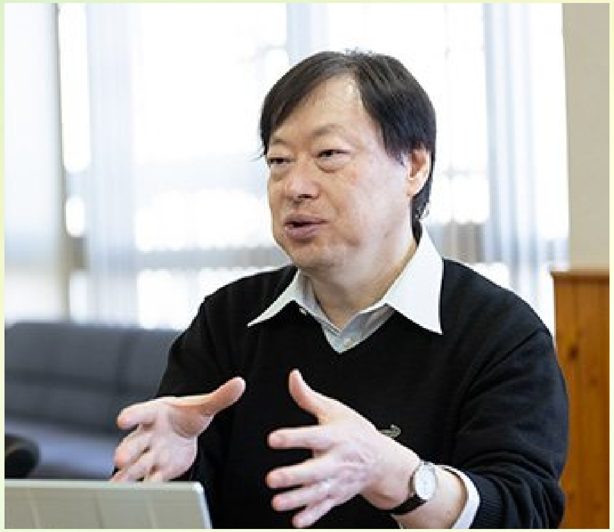
*1 : Abbreviation for “Green Growth Strategy through Achieving Carbon Neutrality by 2050.” This refers to Japan’s industrial policy to connect the challenge of achieving “Carbon Neutrality by 2050” announced in October 2020 with the “virtuous cycle of the economy and the environment.” Among the 14 sectors expected to grow is the Hydrogen, Fuel Ammonia Industry.
https://www.meti.go.jp/english/policy/energy_environment/global_warming/ggs2050/index.html

About the
Researcher



Dr. Okumura is a longtime science enthusiast, having enjoyed experimenting since he was a child. He was fascinated by experiment kits that came with science magazines, often contemplating questions like, “Why does burning charcoal glow a bright orange color? Why does it keep burning?” Growing up during the period of Japan’s high economic growth, Dr. Okumura questioned environmental aspects, wondering, “Is it okay to emit so much CO_2? Can forests alone absorb it? Is the Earth large enough to dilute all this CO_2? Is it acceptable to leave Osaka’s rivers with their unpleasant odor and stagnation as they are?” With such thoughts, he chose to major in comprehensive energy engineering, focusing on research into combustion that does not produce pollutants. As he matured, Dr. Okumura learned about the adverse global effects of indiscriminate CO_2 emissions and, considering industrialization, dedicated himself to the research of CO_2-free burners. The background to his research approach reflects his childhood aspirations.

Associated Research Projects:

- Development of CO_2-free combustor for high intensity combustion and NOx reduction with simultaneous function (hp200033)
- Development of ammonia burner for high intensity combustion and NOx reduction with simultaneous function (hp200176)
- Optimization design of ammonia burner for CO_2-free combustion (hp210108)
- Optimization design of ammonia burner for a carbon-free society (hp220009)

Principal Investigator: Yukihiko Okumura, Kagawa University

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