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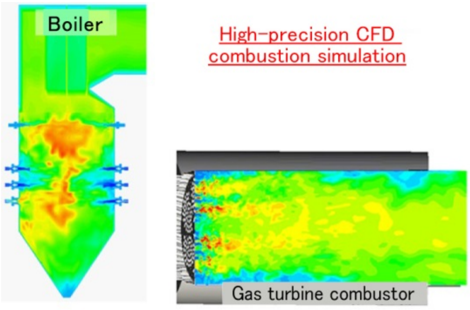
High-precision Combustion Simulation Technology Supporting Energy Transition of Thermal Power Plants



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Mitsubishi Heavy Industries, Ltd. (MHI) has been developing thermal power generation systems burning carbon-free fuels, such as hydrogen, ammonia, etc., to achieve a carbon-neutral society. For the transition to carbon-free fuels, the development of combustion equipment (e.g., gas turbine combustors and boilers) is important. We have been utilizing high-precision combustion simulation technology as a design support tool in addition to combustion tests using elemental burners and actual combustion equipment. This report presents an overview of the high-precision combustion simulation technology that supports the energy transition of thermal power plants, as well as its verification and application examples.

1. Introduction

MHI has been promoting the energy transition of thermal power generation systems toward the achievement of a carbon-neutral society, and has formulated a roadmap shown in **Figure 1**. Specifically, we are developing gas turbines capable of co-firing or single-fuel firing of hydrogen or ammonia, and boilers capable of ammonia co-firing. Since these carbon-free fuels are significantly different from existing fossil fuels in combustion characteristics such as burning rate, the fuel transition for decarbonization requires combustion equipment design that achieves both high reliability and low emissions. Development process based on combustion tests is expensive and time-consuming, and also suffers from the difficulty in understanding the complicated multi-physics coupled phenomena. Therefore, the high-precision combustion simulation technology developed and verified for natural gas-fired gas turbine combustors and coal-fired boilers are further improved/extended considering the difference in combustion characteristics, to support the design of combustion equipment burning carbon-free fuels.

This report presents an overview of the combustion simulation technology as well as its verification and application examples.

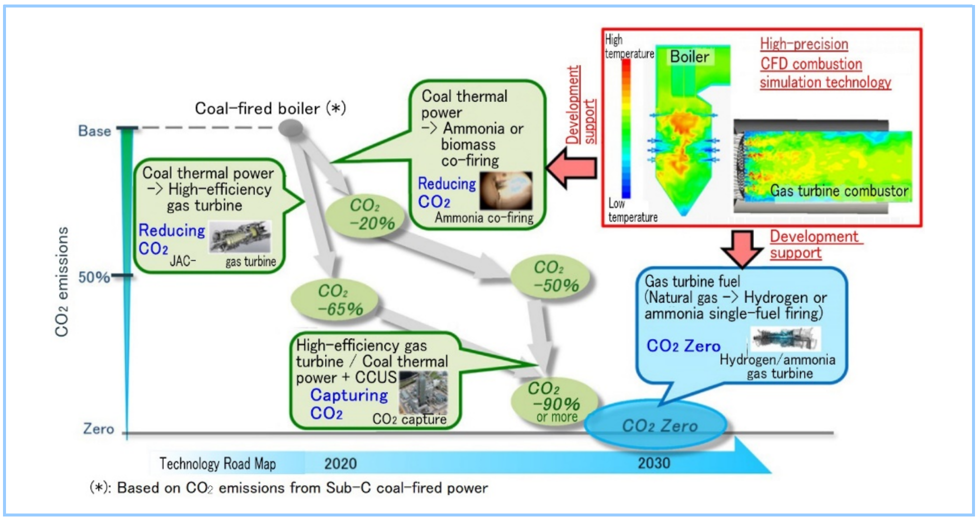

Figure 1 Roadmap for energy transition of thermal power generation systems

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2. Gas turbine combustor combustion simulation technology

Gas turbine combined cycle (GTCC) power generation, as the cleanest power generation system burning fossil fuels, contributes to the reduction of both fuel consumption and emissions. Currently, gas turbines for power generation mainly burn natural gas, and in recent years the fuel transition to hydrogen or ammonia is of a growing need to achieve a carbon-neutral society. Although there are differences in combustion characteristics such as burning rate between the fuels, the important evaluation items for the development of gas turbine combustors are the same in terms of ensuring stable combustion and reducing emissions. The development of combustors that achieve both high reliability and low emissions requires the optimization of design parameters. Since performance verification by combustion tests is highly time-consuming for the design, fabrication, and testing cycles, there is a growing need for design support based on high-precision combustion simulation. This chapter presents an overview of combustion simulation technology applied to gas turbine combustors and its verification and application examples.

The simulation of gas turbine combustors employs the Flamelet approach shown in **Figure 2**, in which the controlling variables (mixing fraction, reaction progress, etc.) characterizing the flame structure are calculated directly in Computational Fluid Dynamics (CFD) simulation, and are used to parameterize all the other physical quantities such as reaction rate, temperature, species mass fraction, etc., by referring to the database based on the detailed chemical reaction mechanism. By simplifying the calculation of detailed chemistry, the Flamelet approach is considered to be a combustion simulation model that is able to achieve both low computational cost and high accuracy (1).

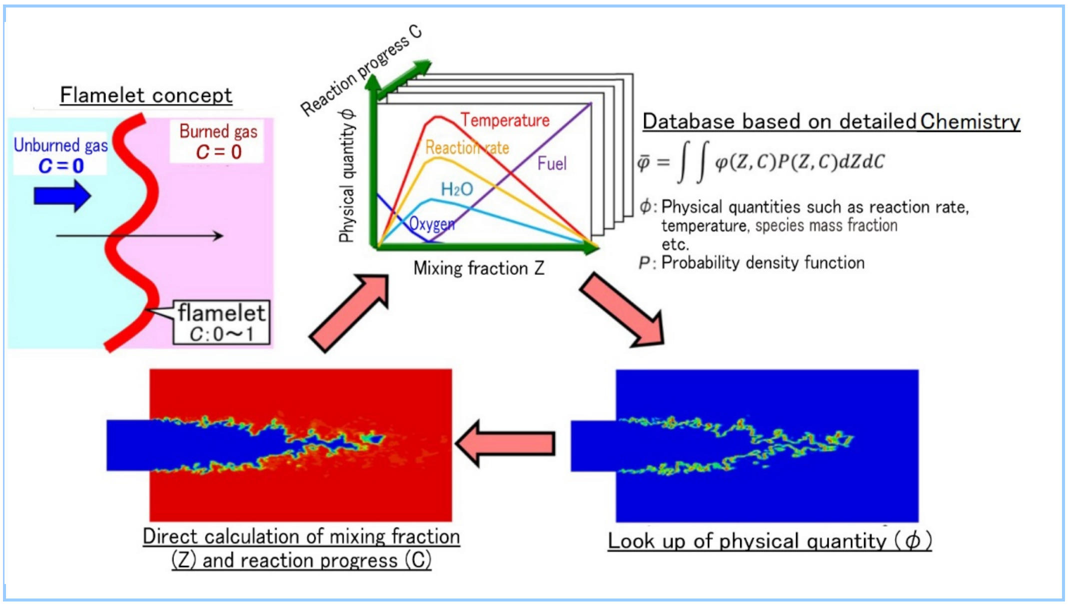


Figure 2 Flamelet approach applied to gas turbine combustors

2.1 Natural gas combustion simulation technology

MHI's state-of-the-art JAC-series gas turbine, with turbine inlet temperature (T1T) as high as 1650℃, has achieved the world's highest power generation efficiency. **Figure 3** shows an overview of the natural gas-fired Dry Low NOx (DLN) combustor in JAC-series gas turbine. In this combustor the premixed combustion method in which fuel and air are premixed before combustion is applied by utilizing the swirling flow.

To accurately predict the flame behavior affected by the highly unsteady turbulent flow in a real combustor (under the conditions of high temperatures, high pressures, and high Reynolds numbers), a Large Eddy Simulation (LES) turbulence model is employed in the numerical simulation. Specific simulation settings such as mesh size, time step, and numerical discretization scheme are optimized based on the measured data of velocity distribution, concentration distribution, temperature distribution, etc.

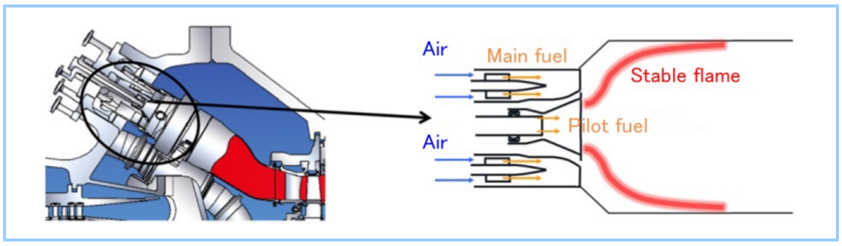


Figure 3 Overview of DLN combustor in JAC-series gas turbine

Figure 4 shows the CFD simulation results of a natural gas-fired combustor. The CFD simulation accurately reproduced the measured flame position (peak position of hydroxyl radical OH* chemiluminescence intensity, bottom left of Figure 4) and temperature distribution (bottom middle of Figure 4) (2). It also well reproduced the trend of changes in nitrogen oxide (NOx) emissions (bottom right of Figure 4) due to changes in the fuel nozzle design. This high-precision combustion simulation technology is currently being utilized as a design support tool for low NOx natural gas-fired combustors.

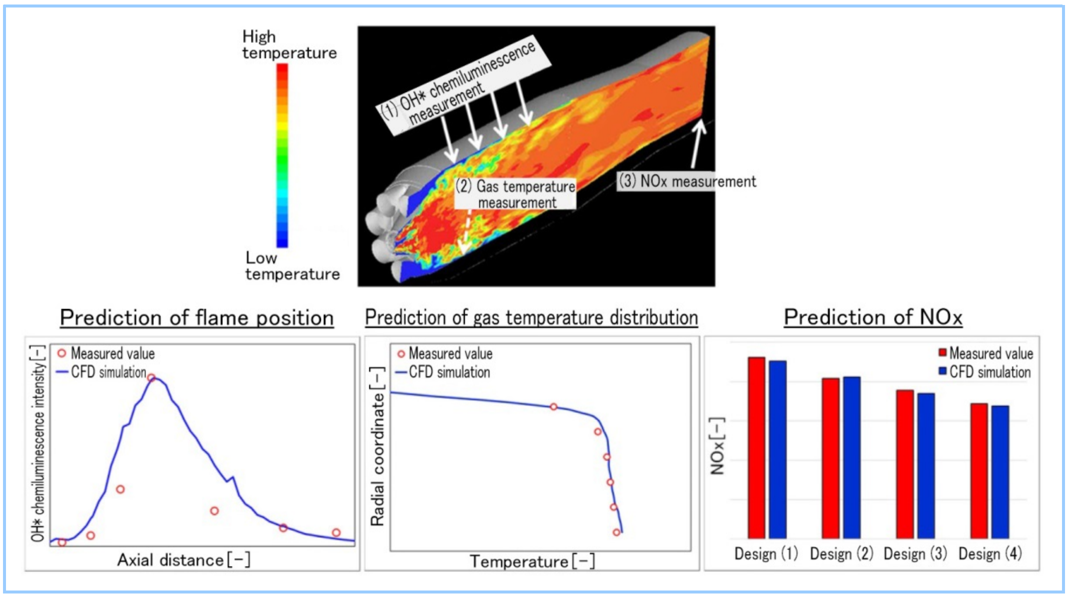


Figure 4 High-precision simulation of natural gas combustion

2.2 Hydrogen combustion simulation technology

With support from the New Energy and Industrial Technology Development Organization (NEDO), we are developing gas turbine combustors capable of hydrogen firing with concentration from 0 to 100%. Hydrogen burns about eight times faster than natural gas, which increases the risk of flashback. Therefore, for the development of the low-NOx emission hydrogen-fired combustor, it is of great importance to guarantee stable combustion preventing the occurrence of flashback. The hydrogen-fired combustor employs the "multi-cluster" concept shown in **Figure 5**(3). The multi-cluster combustor does not use swirling flow for pre-mixing, but mixes air and hydrogen on a smaller scale, aiming for both high reliability and low emissions.

Due to the light molecular weight of hydrogen, the mass diffusion of the fuel is very fast relative to the thermal conduction. The Lewis number (i.e., ratio of thermal diffusivity to mass diffusivity) of natural gas fuel is about 1, but it is much smaller than 1 under high hydrogen concentration conditions. As shown in **Figure 6**, the calculation accuracy of the laminar flame speed (combustion rate) of hydrogen cannot be ensured without considering the Lewis number effect. Therefore, for hydrogen combustion simulation, the Lewis number effect is incorporated into the Flamelet approach.

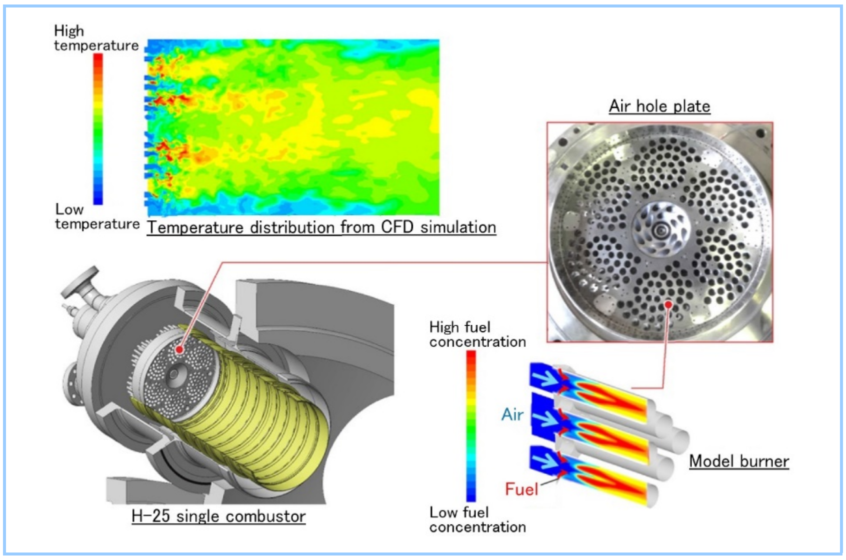


Figure 5 Multi-cluster DLN combustor (hydrogen 0 to 100%)

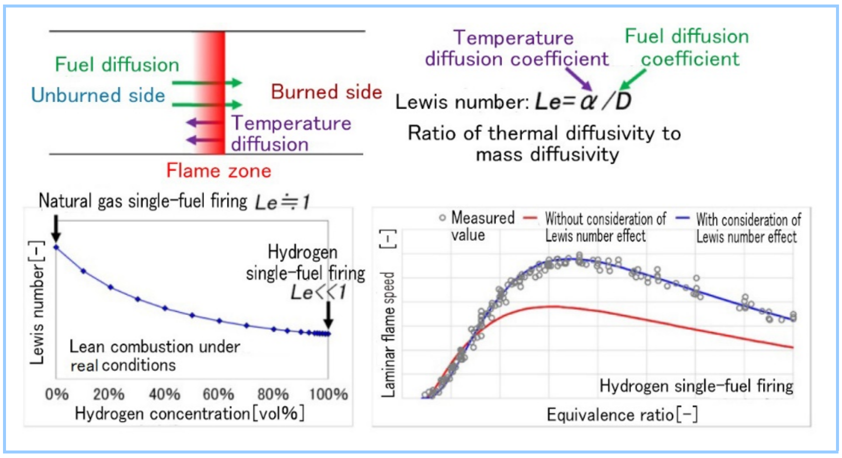


Figure 6 Lewis number effect in hydrogen combustion

Figures 7 and **8** show CFD simulation results of a model burner cut from a full-scale hydrogen combustor. Similar to the natural gas combustion simulation, the CFD simulation reproduced the flame position with a high accuracy. In addition, it also well reproduced the trend of NOx emission changes due to changes in operating conditions and design parameters. These results confirm that this high-precision combustion simulation technology is of the potential to be used as a design support tool for hydrogen-fired combustors.

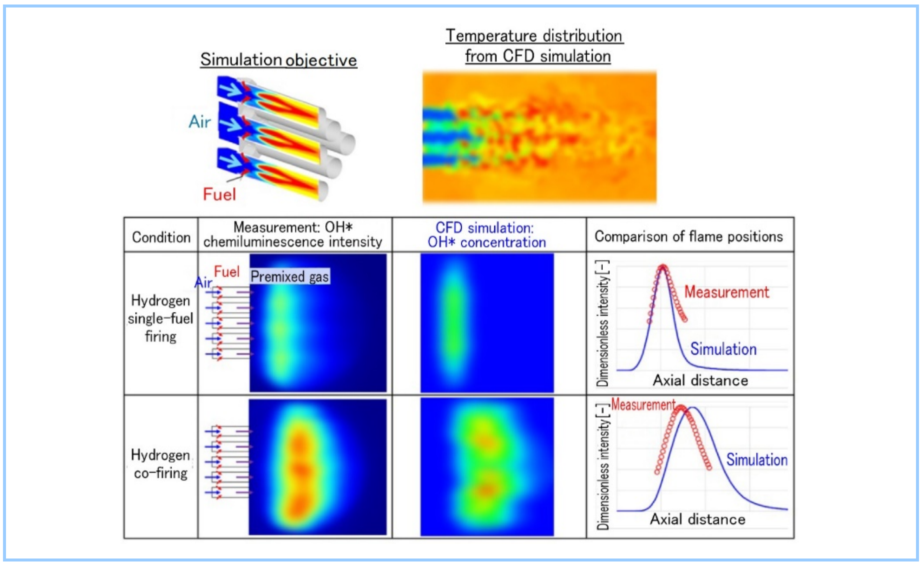


Figure 7 High precision prediction of flame position for hydrogen combustion

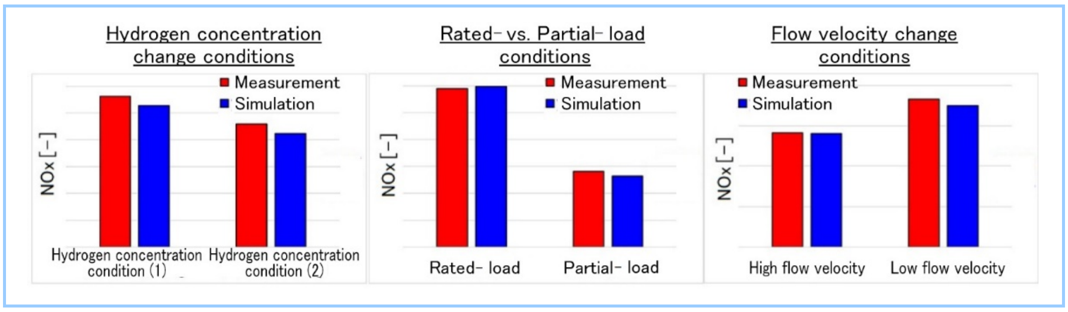


Figure 8 High-precision prediction of NOx for hydrogen combustion

2.3 Ammonia combustion simulation technology

We have started the development of a small-to-medium-size ammonia single-fuel firing gas turbine system. Ammonia burns at about 1/5 the burning rate of methane, which is the main component of natural gas, making it difficult to ensure flame retention. In addition, if the flame is stretched (elongated) by a jet impinging on the wall or by the presence of vortices, the combustion rate is further reduced. If the flame is highly stretched, local extinction may occur, which may lead to flame blowout. At atmospheric pressure, an ammonia flame is extinguished at a flame stretch rate of about one-twentieth that of a methane flame(4), so the effect of flame stretch on stable flame retention is significant. In addition to the difficulty of flame retention, direct ammonia combustion also poses the problem of NOx control. Since NOx emissions can be suppressed when ammonia is combusted in the appropriate fuel concentration range, a lower-NOx combustor can be achieved by optimizing the fuel nozzle and injecting secondary air. If combustion stability and NOx emissions can be predicted with high accuracy using combustion simulation during the combustor optimization phase, the design process will be accelerated.

We have developed ammonia combustion simulation technology that takes into account the effect of flame stretch to predict the stability of ammonia combustion and NOx emissions at the outlet, as shown in **Figure 9**. This technology incorporates the effect of flame stretch on change in burning rate (reaction rate)(5) as a correction factor in the Flamelet approach. We are currently verifying its accuracy in a literature model burner(6), and will apply it as a design support tool for actual combustor in the future.

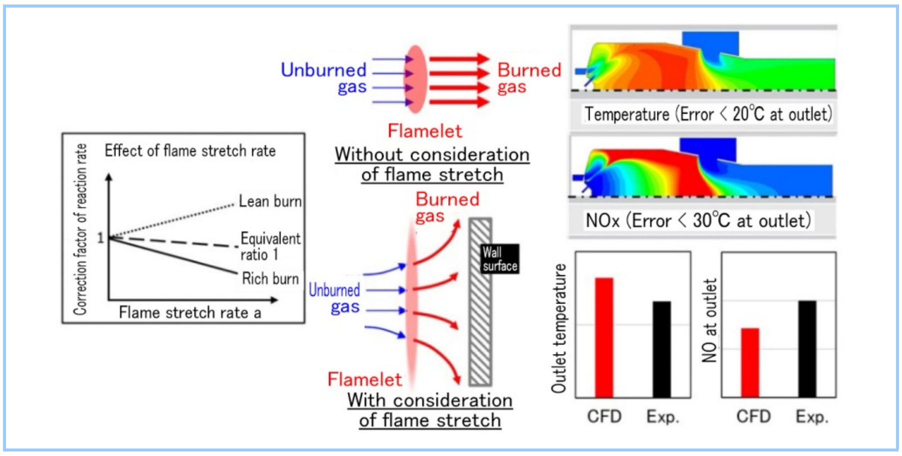


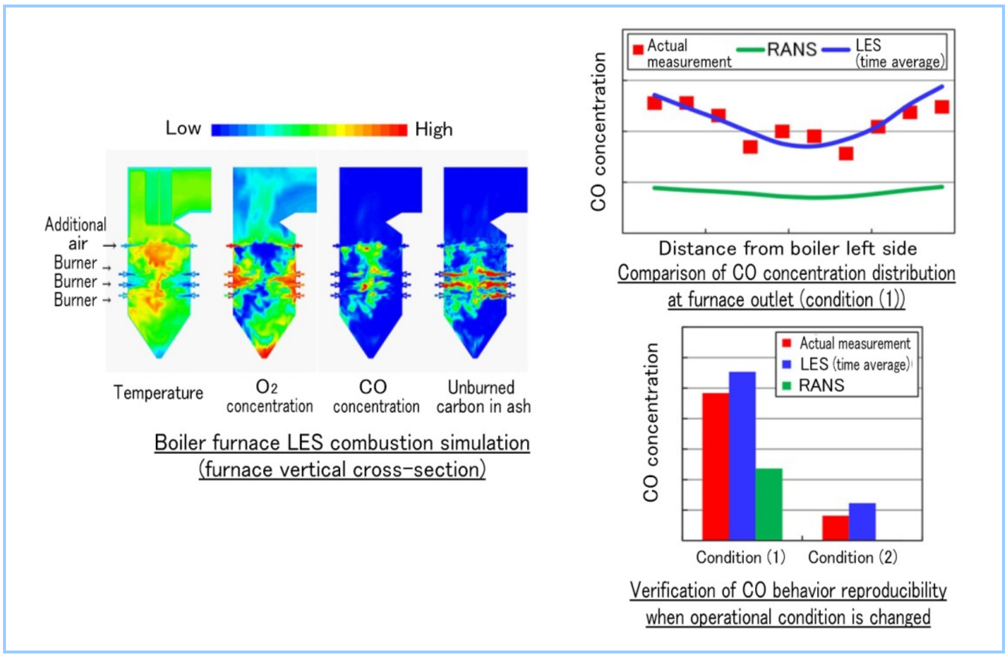
Figure 9 Ammonia combustion simulation considering effect of flame stretch

3. Boiler combustion simulation technology

To enhance exhaust gas performance of a boiler by improving burners and air ports and optimizing operating conditions, it is necessary to understand the combustion conditions in the boiler furnace in detail and accurately evaluate the effect of such improvements and optimizations. It is also important to understand the characteristics of the metal temperature of each part to improve the reliability. We have developed high-precision boiler combustion simulation technology to evaluate the effects of various modifications on various boilers owned by our customers in advance. This chapter introduces examples of verification and application of such boiler combustion simulation technology.

3.1 Coal-fired boiler simulation technology

Boiler combustion simulation is computationally demanding because of the need to incorporate submodels such as pulverized coal behavior and radiation heat transfer, and because of the huge size of the furnace to be calculated. Therefore, in many cases, Reynolds-Averaged Navier-Stokes (RANS) simulation, which is less computationally demanding and assumes a time-averaged field, is used for normal performance evaluation. On the other hand, one of the difficult predictions to be made by RANS is the prediction of carbon monoxide (CO) concentration. One of the factors causing CO is the unsteady heterogeneity in the mixing of pulverized coal and air, which limits the accuracy of prediction by RANS. This section introduces an example of CO concentration prediction by LES, which can simulate non-steady state behavior. **Figure 10** shows an example of LES simulation of an actual boiler. It is observed that the LES can predict the CO concentration at the furnace outlet accurately with respect to the actual measurement, including the CO concentration distribution. The LES can also reproduce the behavior of changes in CO concentration when the air distribution is changed from the condition (1) to the condition (2) with higher accuracy than RANS. This technology can be applied to the development of methods to reduce unburned fuel such as air nozzle modification.



Boiler furnace LES combustion simulation (furnace vertical cross-section)

Comparison of CO concentration distribution at furnace outlet (condition (1))

Verification of CO behavior reproducibility when operational condition is changed

Figure 10 High-precision unburned carbon prediction

Next, we will explain our approach to reliability assessment through the combustion simulation. The superheater at the top of a boiler furnace is composed of many heat transfer tubes, and its metal temperature is affected by the bias of combustion gas, steam flow rate in the tubes, and other factors. For creep life control, proper control of metal temperature is important, but an approach based on measurement using thermocouples is not realistic in terms of cost, durability, etc. Therefore, we have developed a method for predicting heat transfer tube metal temperatures using coupled simulation of heat transfer from combustion gas to steam inside the tubes. By simulating heat transfer to steam flowing through each tube simultaneously with combustion gas flow outside the tube, it is possible to predict the local metal temperature. **Figure 11** shows an example of a project commissioned by NEDO to obtain metal temperature data from an actual superheater and verify the prediction accuracy. This simulation indicated the circumferential metal temperature distribution in the tube cross-section. The highest metal temperature among the measurement points was at the point (a) in both the actual measurement and simulation results, and the simulation was able to predict with an error of +14.2°C relative to the actual measurement. The order of high and low metal temperatures among the measurement points was also consistent between the actual measurement and simulation results, confirming the effectiveness of this technology. We will apply this technology to further improve the reliability of boilers.

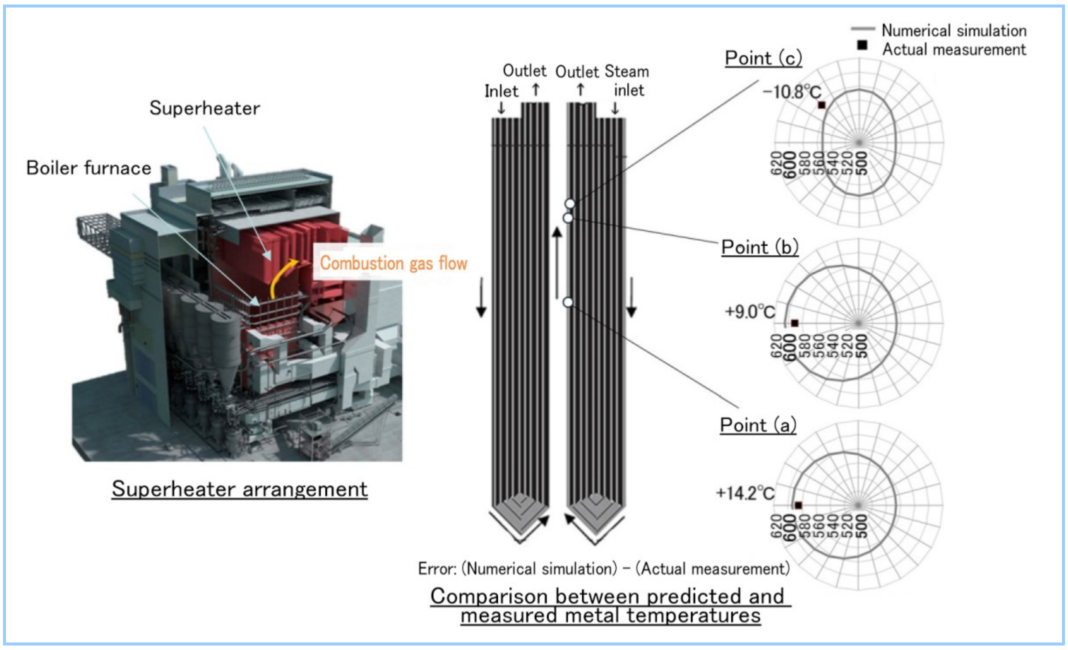


Figure 11 High-precision prediction of heat transfer tube metal temperature

3.2 Coal-ammonia co-firing simulation technology

In recent years, there has been a demand for reducing carbon emissions by coal-ammonia co-firing, and evaluation technology for NOx emissions in the co-firing process is needed. We conducted combustion tests assuming ammonia co-firing in actual equipment using the two-stage drop tube furnace (DTF)(7) shown in **Figure 12**, which consists of an upper stage for reductive combustion of fuel in an air deficient environment and a lower stage for complete combustion with additional air input and can simulate two-stage combustion behaviors in actual equipment, to obtain combustion characteristics data. We developed a NOx model for coal-ammonia co-firing by incorporating ammonia oxidation, pyrolysis, NOx formation, and reduction models into an NOx model for coal firing(8), and verified the model in the two-stage DTF. Figure 12 shows the verification result. It was indicated that the model can accurately predict NOx characteristics even in ammonia co-firing and single-fuel firing.

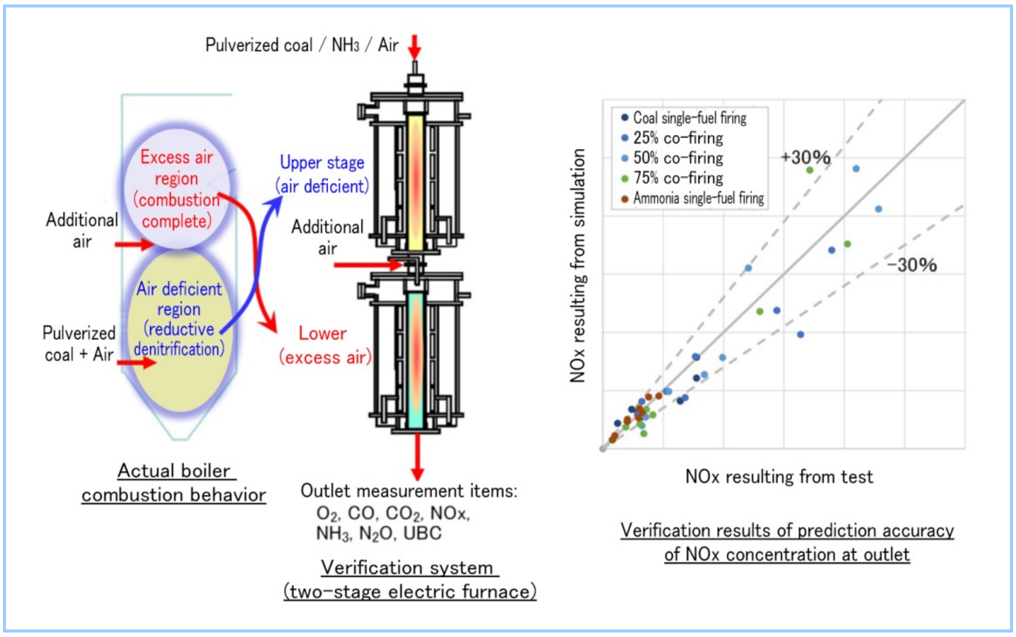


Figure 12 Acquisition of NOx characteristics data and verification of prediction model for coal-ammonia co-firing

Next, this paragraph is introducing an example of the verification of this simulation technology through a small burner ammonia co-firing test (**Figure 13**). In the test, coal and ammonia were co-fired in a dedicated burner for each. The simulation showed that a large amount of NOx was generated near the ammonia burner, but that the reduction progressed thereafter and the NOx generated at the burner section almost disappeared by the time additional air was added. As indicated by the comparison of predicted NOx values at the furnace outlet, the simulation accurately reproduced the NOx behavior in the test. The amount of air to the burner was changed between the ammonia co-firing conditions (1) and (2). The NOx level in the condition (1) was suppressed to the same level as that in coal single-fuel firing, and the test and simulation results were in agreement. It is considered that optimization of air volume is important to suppress NOx levels in co-firing. In the future, we will obtain data from large-scale burner combustion tests, further improve the model and the accuracy, and apply this technology to performance evaluation for modification of actual equipment.

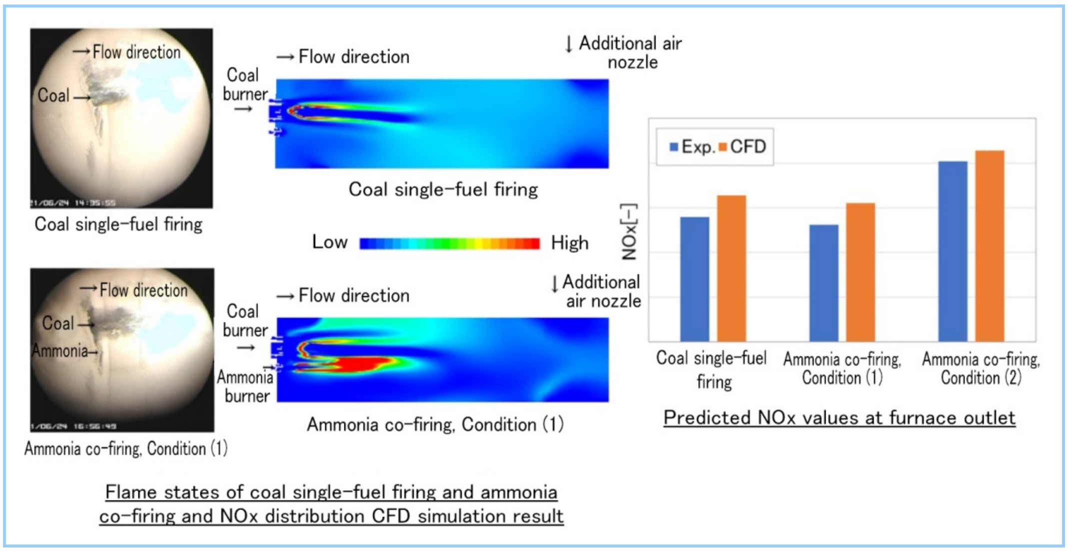


Figure 13 Flame state of coal-ammonia co-firing and accuracy verification

4. Conclusion

This report presented an overview of high-precision combustion simulation technology that supports the energy transition in thermal power plants, as well as its validation and application examples. For gas turbines, the simulation technology verified for natural gas-fired combustors was further improved considering the different characteristics of carbon-free fuels, and reproduced the flame positions and NOx emissions of hydrogen or ammonia combustion with a high accuracy. For boilers, the simulation technology verified with actual coal-fired boilers was further extended based on the basic data of ammonia combustion, and reproduced NOx emissions of ammonia co-firing and single-fuel firing with a high accuracy. Going forward, we will utilize these technologies in the development of combustion equipment, thereby contributing to the acceleration of energy transition.

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