Numerical Prediction of Turbulent Combustion Flows for 1700°C Class Gas Turbine Combustor

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This work simulates unsteady characteristics in a new concept combustor for the 1700 degC class gasturbine in next generation by a large eddy simulation (LES) of turbulent combustion flow. For simulating its new concept of combustion combined with the lean and rich fuel conditions, a 2-scalar flamelet approach developed by the author and his collaborators is applied, where a G-equation model and a conserved scalar model express a propagation of premixed flame and a diffusion combustion process, respectively. These LES and flame models have been conducted successfully on the unstructured FVM code "FrontFlow". Partial premixed reactions in a high Reynolds number turbulence can be explained by the LES and 2-scalar flamelet approach modellings. Temperature profiles in different fuel conditions agree with the measurements essentially. A thermal NO production is also predicted by the detail chemical reaction with Zeldovich's mechanism. For improving some remained discrepancies, a very high resolution calculation with 30 million orders of elements is to be performed.

Keywords: Combustion flow, Turbulence, Gasturbine, Large eddy simulation, Flamelet approach

1. Introduction

Considering environmental issues, regulations of the emissions from combustion systems, such as those of thermal power plants, continue to be tightened, and a higher efficiency of the systems also continue to be desired. To construct a high performance gasturbine combustor for the next generation, some conflicting demands have to be satisfied at high levels. A higher temperature at a combustor outlet is thermodynamically favored for the system efficiency, though a lower temperature is required to reduce a local NOx generation. Therefore, in order to design a high performance gas-turbine combustor satisfying the both criterion, it is very important to obtain a deeper level of understand regarding the phenomena that occur instantaneously and locally in the combustor.

Within these decades, progresses of turbulent combustion modelling have realised a simulation of turbulent combustion flow in a practical combustor. A large-eddy simulation (LES), which is one of the modelling methods of turbulent phenomena, is now expected to act as a powerful tool for more accurate prediction of the practical turbulent combustion flow field. In LES, large vortexes are directly simulated on computational grids and the turbulent effects only in a smaller scale than the computational grids are modelled by sub-grid scale (SGS) turbulent model. Thus, it can be expected that the construction of an interaction model between turbulence and combustion becomes easier and the model effect becomes smaller than the turbulent models based on Reynolds-averaged Navier-Stokes equation (RANS) method. Though the LES requires a high computational cost to simulate time series variations and to average them statistically for getting results, rapid growth of computer technology encourages the realisation of practical LES in a gasturbine combustor geometry.

For a LES of turbulent combustion flow, some reaction models have been coupled with the LES of turbulent flow field. The flamelet approach (*e.g.* Peters 2000) based on the laminar flamelet concept is suitable for coupling with LES because both methods treat the multi-scale phenomena separating into the different scales. Two typical combustion states, which are premixed and non-premixed combustions, are modelled in the different flamelet models for each state. In order to treat more practical situation that includes both combustion states, these combustion models were combined and have been validated in simple geometries (*e.g.* Pitsch *et al.* 2002, Hirohata *et al.* 2003). Recently, a few LES's in practical combustors (*e.g.* Eggenspieler and Menon 2004, Nakashima *et al.* 2007) have also been conducted. These shows that the LES coupled with the flamelet approach can be expected as a practical prediction tool to help combustor designing in the near future.

The present study is performed for the validation of these simulation models of turbulent combustion flows in a practical combustor system; a new concept combustor for the

1700 degC class gasturbine in next generation (Saito *et.al.* 2007).

2. Objective and Numerical Method

A target of this work is a new concept combustor designed by Mitsubishi Heavy Industries for the 1700 degC class gasturbine in next generation, which enable an optimized combustion by controlling the mixture rate of a lean premixed gas from the upstream swirl vanes and a rich one from the side scoop nozzles. For the reacting flow simulations, the LES code "FrontFlow/red ver. 3.0," which is based on the unstructured FVM, had been modified and employed. The two flamelet scalar *G* and ξ-equations,

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{\xi} + \frac{\partial}{\partial x_j}\bar{\rho}\tilde{u}_j\,\tilde{\xi} = \frac{\partial}{\partial x_j}\left(\frac{\mu_{SGS}}{Sc_{SGS}}\frac{\partial\tilde{\xi}}{\partial x_j}\right) \tag{1}$$

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{G} + \frac{\partial}{\partial x_j}\bar{\rho}\tilde{u}_j\,\tilde{G} = \frac{\partial}{\partial x_j}\left(\frac{\mu_{SGS}}{Sc_{SGS}}\frac{\partial\tilde{G}}{\partial x_j}\right) + \rho_u\,S_{SGS}\left|\nabla\tilde{G}\right| \tag{2}$$

are introduced into the code and they can be solved simultaneously with the mass and momentum equations (Nakashima 2007).

The computational domain is shown in Fig. 1 as a computational grid system that is constructed by about 5,942,466 hexagonal elements. The 2nd order Crank-Nicolson scheme is applied to the time integration of the governing equations. A convection term in the momentum equation is discretized by a blending scheme based on a 2nd-order central scheme blending with 10% 2nd-order up-winding scheme. Convection terms in the scalar equations of *G* and ξ are discretized by a 3rd order up-winding scheme with TVD-limiter. The other terms are estimated by the 2nd-order central scheme.

According to the experiments, the following conditions are applied;

Static Pressure in Chamber: 104.35 [kPa]
Inlet gas temperature: 890.3[K] (617.15[°C])
Outlet gas temperature: 1700 [°C]
Fuel components: CH_4 87%, C_2H_6 8%, C_3H_8 5%
Oxidizer components: O_2 13%, N_2 75%, CO_2 6%, H_2O 8%.

Two typical conditions, Lean-Lean mode (L.L.) and Rich-Lean mode (R.L.) are investigated. Developed solutions are obtained after approaching calculation with 20,000time-steps (L.L.) and 60,000 time-steps (R.L.). Time averaged profiles are conducted by 30,000 time-steps (0.075[sec]) for (L.L.) and 12,000 time-steps (0.03[sec]) for (R.L.).

3. Calculation results

Instantaneous temperature profiles in the two difference conditions are shown by the central section views in Fig. 2. It corresponds to mixture rate profiles in a most regions except for the inlets of vanes and side nozzles applied with an unburnt condition. At L.L. mode almost uniform profile is predicted, while at R.L. mode a low temperature zone is observed in the center of the scoop nozzles. In both case, other low temperature regions appear in the downstream of scoop jets due to their wakes. Time averaged temperature profiles from these calculations shown in Fig. 3 agree well with the experimental data measured in the several sections, except for the regions near the inlet vanes.

Next for predicting a NO production rate, a simulation by the detail chemical reaction model is performed, where 27 spices (N2, OH, C3H8, H2, H, CH4, CH3, CH2O, HCO, CO2, CO, O2, O, HO2, H2O, HCCO, C2H2, C2H3, C2H4, C2H5, CH3O, C3H6, iC3H7, nC3H7, N, NO, C2H6), and their 34 reactions are considered. Temperature, density and

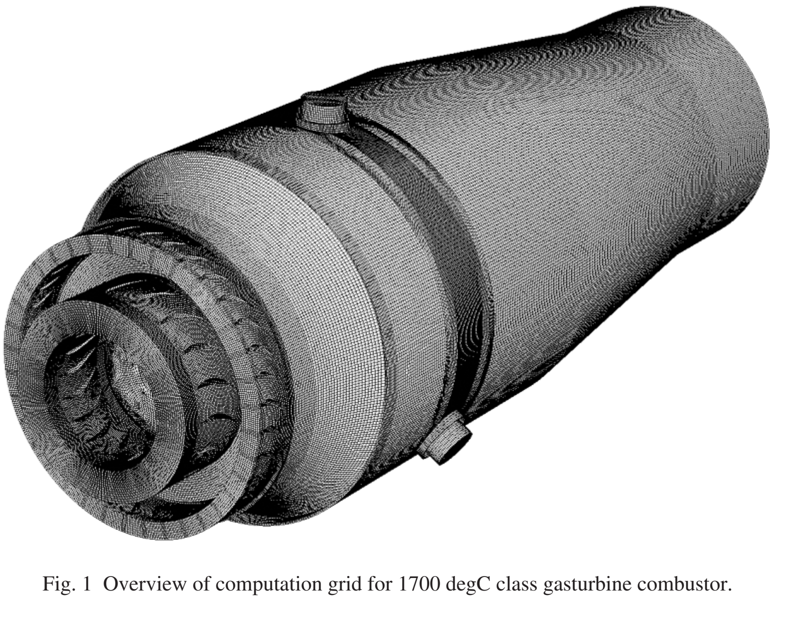

Fig. 1 Overview of computation grid for 1700 degC class gasturbine combustor.

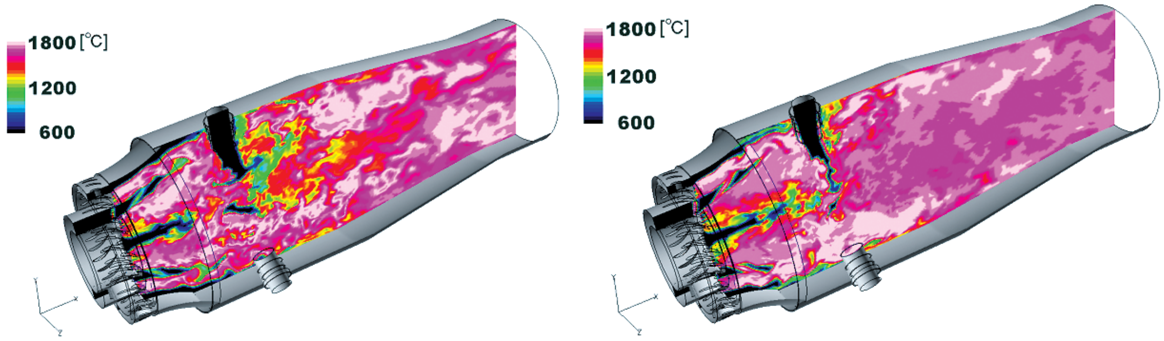

Fig. 2 Instantaneous temperature profiles; left (R.L.), right (L.L.).

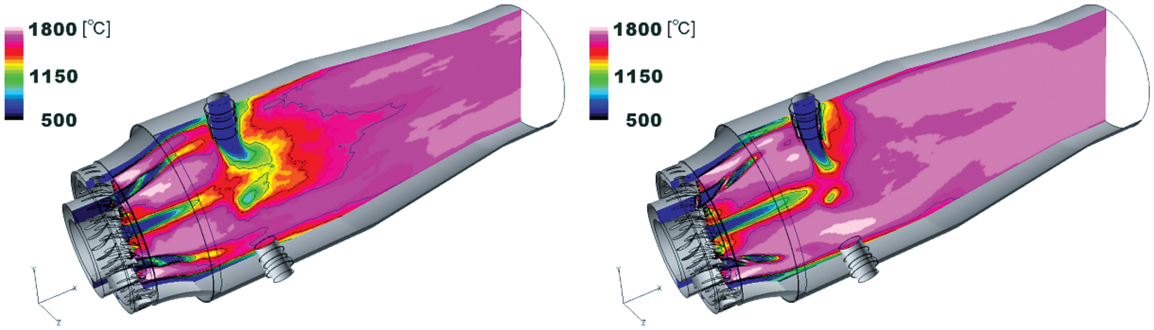

Fig. 3 Time averaged temperature profiles; left (R.L.), right (L.L.).

all spices fraction components at the initial condition are estimated by the above calculation by the flamelet approach. It may give an appropriate condition so that the calculation is performed smoothly after switching the model. Profiles of the NO production rate at the initial (72,000 step) and later times are shown in Fig. 4. Since a time increment is 1/100 smaller than in the previous flamelet approach, there is very little changes of a flow field within the calculation time. After switching the model, the temperature profile changes slightly, but it doesn't influence the NO production so much.

In the present calculations, there are still differences in the region close the inlet vanes, where the velocity fluctuation profile and the fuel distribution by the spray injectors is hardly simulated because the geometry resolution is limited even by this large size calculation with over 5 millions of elements. Therefore more detail resolution with 30 millions of elements is applied to improve the prediction accuracy and reliability.

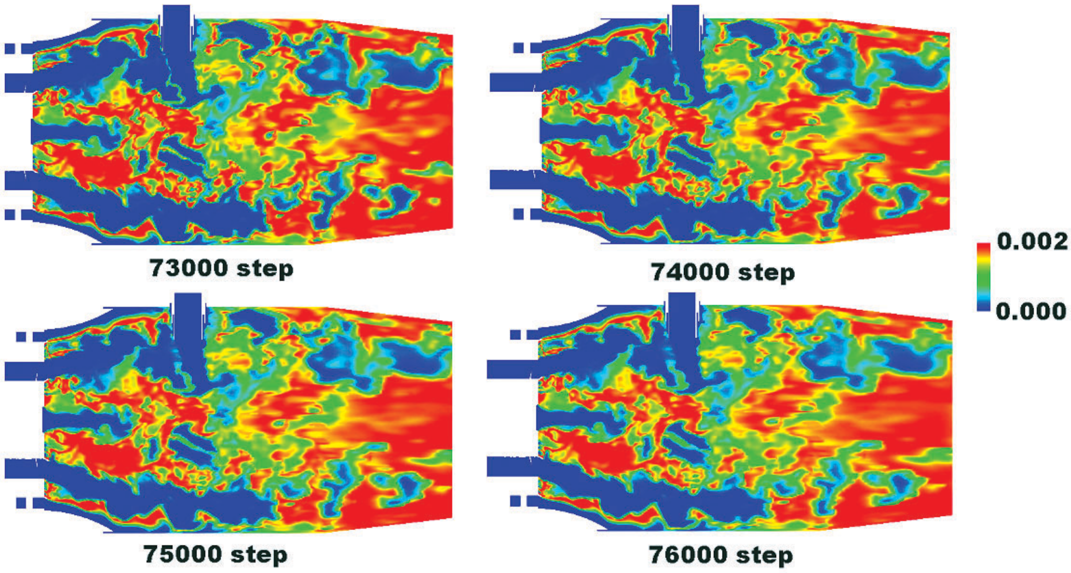

Fig. 4 Profiles of NO production rate predicted by detail chemical reaction.

4. Conclusive remarks

This work exhibits the LES of turbulent combustion flow for a practical combustor system. It validates the feasibility of the 2-scalar flamelet model for such a realistic design of gas-turbine combustor. The software "FlontFLow" (ver.3.0) developed for this work can be excused by upper than 95% vector processing ratio and super-linear (efficiency over 1) acceleration with 32 to 80 CPUs on the earth simulator system.

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本研究では1700°C級次世代ガスタービン燃焼器の乱流燃焼場の非定常予測として大規模なラージ・エディ・シミュレーション(LES)を開発、実行した。実機燃焼器における複雑な燃焼状況の予測のため、著者らが開発した2スカラー火炎片近似(flamelet approach)モデルを採用し、数値計算には非構造格子に適合した汎用流体解析ソフトウェアFrontFlowを適用した。ここでは層流火炎片近似に基づき、予混合伝播火炎をG方程式により、拡散燃焼火炎を混合分率の保存スカラー式によりそれぞれモデル化され、乱流LESの体積平均近似において定式化されている。これによって、高レイノルズ数の部分予混合燃焼の実用解析が可能となった。ガスタービン燃焼器の異なる燃料条件における温度予測は実験結果の基本的な特徴を良く再現している。また、詳細反応モデルを用いてZeldovich機構による温度NOの生成率予測も得られた。今後、超大規模計算格子(3000万要素規模)を適用して形状および燃料流動条件の詳細を再現することによる予測精度改善を図っている。

キーワード: 燃焼流, 乱流, ガスタービン, ラージ・エディ・シミュレーション, 火炎片近似