Numerical analysis of the effect of the hydrogen composition on a partially premixed gas turbine combustor

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A B S T R A C T

Large-eddy simulations (LESs) of a hydrogen-enriched 1/3-scale GE7EA gas turbine combustor are conducted. Four different fuel compositions are employed to investigate the role of the CH4/H2 syngas composition on the resulting flame structure and pressure oscillations occurring inside the combustor. A comparison with the experimental data is conducted to validate the numerical results. First, imaging processing is performed using an Abel-inversion technique for the accumulated OH mass fraction showing good agreement with the experimental images. Then, the calculated velocity fields are successfully compared to the experimental (particle image velocimetry) results. The results show that the flame structure is readily altered when changing the syngas composition; this strongly affects the flow field and therefore the pressure oscillations inside the combustor. When the hydrogen composition is increased, the flame becomes shorter and thicker, and its effect on the outer recirculation zone is minimized. When the flame length approaches the radial length of the combustor under certain conditions, the flame periodically attaches to the rigid wall and the pressure oscillations inside the combustor become amplified. Overall, the LES combined with the multi-step kinetics successfully predicts the variation in the flow fields due to fuel composition changes and reveals the role of the syngas composition in the combustor.

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Introduction

Syngas is a fuel gas mixture consisting primarily of H2, CO, and CH4 and is a promising alternative energy source that can improve the overall performance and replace natural gas in the operation of a gas turbine. The characteristics of syngas, such as its lean blowout limits, flame structure, and emission, have been widely studied over the last few decades [1].

Of these characteristics, the hydrogen enrichment effect in hydrocarbon fuels has constituted the primary research focus due to its positive characteristics with regard to the combustion stability and emission reductions. Previously, Schefer et al. [2] investigated the effect of hydrogen enrichment on the increase in the flame blowout limit in lean conditions as well as the reduction of CO emissions without increasing NOx emissions in a premixed burner. Cozzi et al. [3] studied how hydrogen addition affects the operation of a natural gas non-premixed burner via a shorter and narrower flame while the stability limits were increased in the hydrogen-enriched condition. In addition, previous experimental studies have...
indicated that alterations in the hydrogen ratio in syngas significantly influence the flame structure and flow fields. Emadi et al. [4] investigated the effect of the hydrogen composition on the flame structure generated by a premixed methane-air burner and showed that hydrogen enrichments in the burner significantly increased the flame surface density and the blowout limits. In addition, Hong et al. [5] investigated how hydrogen enrichments affect the recirculation zone in a reactive swirling flow and the overall flame structure including the blowout phenomenon.

However, attempts to properly simulate a hydrogen-enriched flame in a combustor have remained ongoing [1] and only a few studies have considered this issue. De et al. [6] conducted an LES study of an unconfined swirling burner, and the effect of parameters including the hydrogen composition on the upstream flame propagation was investigated. In addition, Hernandez-Perez et al. [7] conducted LESs under hydrogen-enriched conditions and measured the flame structure and emission effect of hydrogen enrichments. Direct numerical simulations (DNSs) of hydrogen-enriched methane flames have also been conducted to investigate the role of hydrogen on the flame characteristics [8]. Nevertheless, a more in-depth investigation is necessary because detailed simulations and validations of flow fields for various hydrogen compositions are limited and an attempt to connect the hydrogen composition to unstable pressure responses in combustors needs to be presented. Therefore, we focus on the accurate reproduction of a hydrogen-enriched flame to analyze the effect of fuel composition on the flow fields and pressure oscillations.

Several previous studies have conducted experiments on fuel composition effects in combustors. An experimental study by Allision et al. [9] indicated that variations in the operating fuels altered the instability amplitudes and frequencies not acoustically derived from the closed combustor geometry. Their results also demonstrated that the oscillation frequency is proportional to the fuel flame speed while the oscillation magnitude remains relatively unchanged for various hydrocarbon fuels. However, the study by Lee et al. [10] revealed slightly different characteristics. While the laminar flame speeds of various syngas compositions behaved similarly in terms of their oscillation frequencies, the fuel composition effects on the pressure oscillation results were very distinct. In Ref. [9], the three types of hydrocarbon fuels studied presented similar amplitudes while the hydrogen-enriched carbon monoxide showed a weaker oscillation magnitude. In Ref. [10], no prominent oscillations were observed in the pure hydrocarbon fuels (methane and carbon monoxide) because their oscillation magnitudes were too low. Rather, only the hydrogen-enriched hydrocarbon syngas resulted in a strong combustion instability.

Accordingly, a reliable numerical prediction of the related flow field in a gas turbine combustor, which takes into account the various operating conditions and in particular the hydrogen effect in the interior flame structure and flow fields, is highly desired. In addition, in this study, the effect of the syngas composition on the magnitude of the oscillation is investigated while seeking an explanation for the above-mentioned issues. A detailed verification procedure is pursued with a series of validation calculations that include the reaction mechanism, which consists of 15 species and 23 reaction steps for comparison against the measured flame speed. Then, the complex turbulent reacting flow in a model gas turbine combustor is simulated and the results are compared to experimental measurements [11].

**Experimental setups**

The model gas turbine combustor, shown in Fig. 1, was used to study the effect of the fuel composition on the instability phenomenon. The combustion of air at 200 ± 5 °C controlled by a mass flow controller (MFC) was supplied via a central annular swirling nozzle, and 90% of the area of the combustor outlet was blocked via a water-cooled plug nozzle to achieve an acoustic boundary at the combustor outlet. The uniformity of the fuel mixture was acquired via an inline mixture, and well-mixed fuel was injected into the combustor through 14 fuel holes within the inner side of the swirl vanes 2.7 mm upstream of the dump plane to form a partially premixed flame. A detailed picture of the dump plane and the swirl nozzle is given on the right side of Fig. 1. A total of 11 dynamic pressure sensors (PCB-102A05) and 4 k-type thermocouples were used to measure the unsteady phenomenon and control the inlet air temperature. The measurement units of pressure sensors and thermocouples are in psi and Kelvin. DAQ module was used to convert the digital signal to an analog signal and LabVIEW was used to acquire the data. The fuel composition, airflow rate, and equivalence ratio were selected as the main variables. The particle image velocimetry (PIV) technique was adapted to obtain the flow field during the reacting condition.

![Fig. 1 – A 1/3-scale GE7EA model gas turbine combustor.](image-url)
An extrapolation technique was additionally used to compensate for the accuracy of PIV near the wall. An ND-YAG laser was used for the PIV, and the scattering signal was measured via a CCD camera, lens, and band pass filter. The PIV and OH-chemiluminescence measurements were taken in the combustor to measure the flow fields and the flame structures of the swirling turbulent flames.

**Numerical details**

**Governing equations**

In this study, large-eddy simulations (LESs) were performed using the finite volume method for the spatial integration with an open-source CFD tool, OpenFOAM [11]. In particular, the unsteady compressible combustion solver, reactingFoam, was adapted in this study. For low-Mach number solutions requiring pressure closure, the well-known PIMPLE algorithm was used. The resulting compressible governing equations of mass, momentum, energy, and species for the given reacting flow are as follows.

\[
\frac{\partial}{\partial t} (\rho) + \frac{\partial}{\partial x_i} (\rho u_i) = 0
\]

(1)

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial}{\partial x_j} (\rho \mathbf{u} \cdot \mathbf{f}_i) + \frac{\partial}{\partial x_j} (\mu_t \frac{\partial u_i}{\partial x_j})
\]

(2)

\[
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_i} (\rho u_i e) = - \frac{\partial}{\partial x_i} (\rho u_i u_j) + \frac{\partial}{\partial x_j} \left( k + \mu_e \frac{\partial e}{\partial x_j} \right)
\]

(3)

\[
\frac{\partial}{\partial t} (\rho Y_i) + \frac{\partial}{\partial x_j} (\rho u_j Y_i) = \frac{\partial}{\partial x_j} \left( D \frac{\partial Y_i}{\partial x_j} \right) + \mathbf{u}_i
\]

(4)

Here, \( \rho \) is the filtered density, \( \mathbf{u} \) is the Favre-filtered velocity, \( \mathbf{E} \) is the Favre-filtered total energy, \( Y_i \) is the Favre-filtered mass fraction, and \( \mathbf{w}_i \) is the filtered sensible enthalpy. The turbulence properties \( \mu_t, Pr_t \), and \( Sc_t \) are the turbulence viscosity, the turbulence Prandtl number, and the turbulence Schmidt number, respectively. The fluid properties \( \mu, k \), and \( D \) are the viscosity, the thermal conductivity, and the molecular diffusivity, respectively. In the LES framework, relatively large-scale motions are directly solved and small-scale motions are modeled using a subgrid-scale stress model. In this study, the subgrid-scale modeling was performed using the WALE model [12]. The subgrid-scale viscosity is described using the following equations.

\[
\nu_{sgs} = C_s \Delta \sqrt{k_{sgs}}
\]

(5)

\[
k_{sgs} = \left( \frac{C_s^2 \Delta}{C_k} \right)^2 \frac{\left( S_s^p S_s^m \right)^3}{\left( S_s^p S_s^m \right)^{5/2}} \left( \frac{S_s^p}{S_s^m} \right)^{5/4}
\]

(6)

\[
S_s^p = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

(7)

\[
S_s^p = \frac{1}{2} \left( \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} \right) - \frac{1}{3} \left( \frac{\partial \tau_{ii}}{\partial x_i} \right)
\]

(8)

Here, \( C_s \) and \( C_w \) are the model constants, which are fixed at 0.17 and 0.325, respectively. \( k_{sgs} \) is the subgrid-scale kinetic energy, \( S_s^p \) is the filtered strain rate tensor, and \( \mathbf{w}_i \) is the velocity gradient tensor.

**Chemistry model**

In the presented simulation, accurate calculations of the flame length and flame structure, as well as the OH profile, in comparison with the experimental data are key factors in the analysis of the dynamics of the combustor flow. Accordingly, a 23-step reduced chemical kinetic scheme consisting of 15 species [13] was implemented to calculate the hydrogen-enriched methane flame. The kinetics of this scheme was verified prior to a full combustor simulation for the laminar flame speed. We calculated the 1D laminar flame speed using the current OpenFOAM solver and verified the chemical kinetics as implemented in the combustion solver. Fig. 2 shows a comparison of the 1D calculation with the experimentally measured laminar flame speed [13] and a reference calculation [13]. The comparison shows that the solver accurately predicts the flame speeds under various pressure conditions. Therefore, the kinetics and solver are suitable for simulating a gas turbine combustor in which the pressure oscillation occurs internally (see Fig. 3).

To simulate the turbulent reacting flow in a gas turbine combustor, the Arrhenius rate law is usually not suitable because the actual reaction rate is nonlinearly dependent on the temperature and species composition and therefore cannot be resolved on LES grids due to their small scales.

\[
\omega_i(\rho, T, Y_j) \neq \omega_i(\rho, T, Y_j)
\]

(9)

To properly handle such a source term, an additional approach, called the turbulence-chemistry interaction model, was adapted. To simulate a partially premixed flame, where the fuel and the air are not fully premixed prior to entering the combustor, the Partially Stirred Reactor (PaSR) model [14] was used. The production rate of a reaction \( i \) is written as follows.

\[
\frac{dc_i}{dt} = \frac{c_i - c_{eq}}{\tau} = \frac{c - c_{eq}}{\tau_{cm}} = f_i(c)
\]

(10)

\[
c_i = c \left( \frac{T}{T + \tau_{cm}} \right) + c^0 \left( 1 - \frac{T}{T + \tau_{cm}} \right)
\]

(11)
Here, \( c_1 \) and \( c_0 \) are the concentrations at the inlet and outlet of the cell, respectively, \( r_i \) and \( r'_i \) are the stoichiometric coefficients, \( \tau \) is the time step, \( t_m \) is the micro mixing time, and \( \dot{w}_i \) indicates the progress rate of the reaction \( i \). Using the above relations, a generalized model can be derived:

\[
f_i(c) = (r'_i - r_i) \dot{w}_i
\]

\[
f_i(c) = f_i(c_1) + \left( \frac{\partial f_i}{\partial c} \right)_{c=c_1} (c-c_1) = f_i(c_1) - \frac{c-c_1}{\tau},
\]

\[
f_i(c) = f_i(c_1) - \frac{c_1 - c_0}{\tau} = f_i(c_1) - \frac{t_c}{t_c + t_m},
\]

where \( t_c \) is the chemical reaction time scale. The chemical source term was determined based on the given chemical interaction model.

**Numerical setup**

In this study, a 1/3-scale GE7EA model gas turbine combustor was selected as the target. In the entrance, the syngas and air are injected through a plug nozzle that has 14 swirl channels (swirl number = 0.832). The mass flow rate of the air was 1100 slpm, and the fuel flow rate was varied according to the composition of the syngas because the heat input of the syngas was fixed to 40 kW [11]. In addition, the oscillation strength in the fuel flow rate varied because the inlet pressure fluctuations were different in each case [15]. The combustion instability associated with the present experiment is self-excited oscillations, which are a confined geometry mode coupled with heat release and fuel flow fluctuations and generate the feedback mechanism of the combustion instability. However, an attempt to calculate the entire process is computationally too

![Fig. 2](image1.png) Verification of the chemical kinetics with the experimental results.

![Fig. 3](image2.png) (a) Schematic of the model gas turbine and (b) the four different mesh sizes used inside the combustor.

| Table 1 – Initial conditions of the simulated cases in various syngas compositions. |
|-----------------|-----|-----|-----|-----|-----|
| Numerical case  | A   | B   | C   | D   | E   |
| H₂ ratio (mole F.) | 0   | 50  | 75  | 100 | 50  |
| Equivalence ratio | 0.573 | 0.552 | 0.529 | 0.48 | 0.552 |
| Air flow rate (slpm) | 1100 |     |     |     |     |
| Mean fuel flow rate (slpm) | 66.2 | 102.0 | 139.8 | 222 | 102.0 |
| Fluctuation mag \( \left( \frac{u}{U} \right) \) | 1/3 | 2/3 | 1/3 | 1/3 | 2/3 |
| Heat input (kW) | 40  |     |     |     |     |
| Radial distance (mm) | 65  | 65  | 65  | 65  | 120 |
expensive [16] when considering the various operating conditions. Henceforth, we assume a forced response where the outlet of the combustor is considered to be an open boundary and analyze the dynamic response characteristics inside the combustor. The experimental pressure and velocity fluctuation data were entered into the simulation, and the considered cases are tabulated in Table 1.

In the nozzle, the fuel and air are partially premixed in a relatively short mixing zone (2.7 mm). The syngas is continually injected through the combustor and generates a swirled flame. In the mixing zone, we used a very fine unstructured mesh of 0.3 mm to properly simulate the incomplete mixing by assigning nine grids in each dimension of the mixing zone. In the combustor, a 2-mm unstructured mesh was used in the flame-generating zone to properly resolve the reacting zone. In addition, a 4-mm unstructured coarse mesh was used in regions where the reaction did not occur.

Fig. 4 – (a) Accumulation of the 3D profiles into a 2D image, (b) the accumulated image, and (c) the Abel-inversion image.

Fig. 5 – Comparison of the Abel-inversion flame images for various fuel compositions.
Results

Flow fields

Images of the simulated time-averaged flames in the gas turbine were compared to the experimental data. In the experiment, an OH-chemiluminescence measurement was conducted at the quartz tube using a high speed ICCD camera to visualize the flame. The frame rate in the measurement was 7000 frame/s, and the recorded image size was $1024 \times 1024$ pixels. The images were recorded for approximately 1 s and were time-averaged to capture the mean values of the flame images. In the time-averaged image, the signal of the OH radicals in the flame was accumulated into two dimensions. In the simulation, the OH mass fraction was

Fig. 6 – Profiles of the time-averaged (a and c) $U_y$ and (b and d) $U_z$ velocity components at various axial locations in (a and b) 75% $H_2$ and (c and d) 50% $H_2$ fuel compositions for the experiments (symbols) and LESs (lines), where $D$ is the axial distance from the dump plane.
calculated and time-averaged. The data were continually integrated along the y-axis to match the experimental conditions (Fig. 4a). The Abel-inversion technique was used on the averaged images in both the experiment and the simulation to capture the 2D flame boundaries and to analyze the flame structures.

To properly implement the imaging process, the three-point Abel method proposed by Dasch [17] was applied using a MATLAB code. The Abel-inversion code reads in the brightness of the accumulated grayscale images (Fig. 4b) and transforms them into the processed images (Fig. 4c). As shown in Fig. 5, the simulation results for the flame length and structure match the experimental results well. In addition, increases in the fuel hydrogen ratio make the flame shorter, which is consistent with the experimental observation. In addition, the shortened flame structure is observed in both simulation and experiment in high hydrogen content due to the higher combustibility and faster flame speed of the hydrogen.

Figs. 6 and 7 show the y- and z-axis distributions of the velocity profiles for 50% H₂ + 50% CH₄ and 75% H₂ + 25% CH₄ composition flames. From the comparison, we can conclude that the simulation results predict the experimental data well, except for Uₖ in the recirculation area. The error in the Uₖ values may originate in the outflow because an open boundary condition is imposed in this region. Unlike the flame shape, the velocity profile remains relatively unchanged with increasing H₂ composition, which indicates that the velocity field in the combustor is primarily influenced by the input airflow rate. In succession, the comparison of the streamline profiles with the PIV measurements is made. The numerical vector profiles were calculated during the simulation and post-processed for the 2D sectional region and the PIV measurement region. The streamline profiles of the combustor and the PIV region are described in Fig. 8.

According to Fig. 8, the streamline fields in two simulation cases (B and C) predict the PIV results very accurately. Because the inlet flow hits the rigid wall and ricochets into two regions, a strong recirculation zone is observed where the flow ricochets into the injectors and circulates inside this region. In addition, a relatively weak and large recirculation zone is observed along the wall surface. The simulation results indicate that some portion of the swirled flow ricochets into the outflow area and forms a large weak vortex along the area of the wall boundary. Unlike in case C, the streamlines in case B progress into a relatively smaller and more wrinkled
recirculation zone, which indicates that the relatively short flame length affects the overall shape in the outer recirculation zone. These results support the numerical and experimental observations in swirled gas turbines in the literature. Meanwhile, the experimental instability characteristics of the above two cases are distinct because the 50% H₂ operating condition results into a strong pressure fluctuation inside the combustor whereas the 75% H₂ operating condition has no oscillation in the combustor (in both the experiment and the simulation). According to Ref. [19], the coupling of the vortices and the flame inside the combustor generally excites such unstable phenomena. Therefore, one can conclude that the strong recirculation zone in case B may be the primary source of the instability in the previous experiment. Because the flame length is highly diversified in each syngas composition in Fig. 5, the effect of the flame structure on the pressure oscillation in the combustor is considered further.

Dynamic response in the combustor

The dependence of the instability characteristics on the syngas composition is considered here. In the results of the simulation shown in Fig. 9, the oscillating flame periodically hits the rigid wall for certain compositions of syngas and the pressure oscillation appears to follow this phenomenon (Fig. 10). Previous experimental study [10] using the same combustor also reported the identical periodic flame attachment/detachment phenomena, which were referred to as the instability driving mechanism. The numerical results in the present work further confirm that finding.

In comparison, when the H₂ composition is close to zero or occupies the majority of the fuel composition, the oscillating flame does not hit the wall periodically due to its flame length. As a result, no strong response in the pressure oscillation is observed. To investigate the effect of geometry on the pressure oscillation, further investigations concerning this phenomenon were performed (case E) in simulations with a combustor with an increased radial length. In contrast to the results in the original geometry, a strong oscillation does not appear at all in the pressure field inside the combustor. The results of the pressure oscillation in each case are shown in Table 2. These results indicate that the interaction of the radial combustor geometry and the fluctuating flame could be the major factor in the strong response of the pressure oscillation in the combustor.

Conclusions

In this study, an investigation of a hydrogen-enriched gas turbine combustor and the effect of the hydrogen composition on a partially premixed gas turbine combustor was performed. An LES using a PaSR model and a reduced chemistry scheme were applied to properly simulate the turbulent reacting flow in a model gas turbine. The experimental measurements for various syngas compositions were used to validate the simulation. In particular, the velocity field results were validated using the PIV results. Then, a flame structure analysis was performed with the integrated OH profiles, and the results were compared to the OH-chemiluminescence images. The comparison indicated that the simulations adequately predict the reacting flow for various syngas compositions, and that the flame structure is greatly altered when the hydrogen composition is changed. A pair of vortices, one smaller and stronger and one larger and weaker, are observed in each case. A comparison with the PIV results indicates good agreement for the vortical structure, and it is shown to vary largely depending on the fuel composition. When the hydrogen composition is approximately 50%, a stronger, larger outer recirculation zone and a periodic attachment of the flame to the rigid wall are found, and the response of the pressure oscillation is greatly increased in these regions. Therefore, this study confirms that the flame structure and recirculation zones, which are strongly affected by the syngas

<table>
<thead>
<tr>
<th>Numerical case</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂ ratio (mole %)</td>
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<td>50</td>
<td>75</td>
<td>100</td>
<td>50</td>
</tr>
<tr>
<td>Oscillation mag. (Experiment)</td>
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<td>1020</td>
<td>52</td>
<td>41</td>
<td>—</td>
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<tr>
<td>Oscillation mag. (Numerical)</td>
<td>152</td>
<td>682</td>
<td>76</td>
<td>30</td>
<td>48</td>
</tr>
</tbody>
</table>

Fig. 9 – Unstable flames (case B) shown via the temperature field for four different phase angles.

Fig. 10 – Dynamic pressure profiles for each fuel composition case.
composition, are important factors for understanding and managing instabilities in a gas turbine combustor.

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References


