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COMBUSTION CHARACTERISTICS OF H₂/N₂ AND H₂/CO SYNGAS
NONPREMIXED FLAMES

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Abstract:

Turbulent nonpremixed $\text{H}_2/\text{N}_2$ and $\text{H}_2/\text{CO}$ syngas flames were simulated using 3D large eddy simulations coupled with a laminar flamelet combustion model. Four different syngas fuel mixtures varying from $\text{H}_2$-rich to CO-rich including $\text{N}_2$ have been modelled. The computations solved the Large Eddy Simulation governing equations on a structured non-uniform Cartesian grid using the finite volume method, where the Smagorinsky eddy viscosity model with the localised dynamic procedure is used to model the subgrid scale turbulence. Non-premixed combustion has been incorporated using the steady laminar flamelet model. Both instantaneous and time-averaged quantities are analysed and data were also compared to experimental data for one of the four $\text{H}_2$-rich flames. Results show significant differences in both unsteady and steady flame temperature and major combustion products depending on the ratio of $\text{H}_2/\text{N}_2$ and $\text{H}_2/\text{CO}$ in syngas fuel mixture.

Key Words: Non-premixed combustion, Syngas, Hydrogen, Carbon Monoxide, Nitrogen, LES, Large Eddy Simulation, Flamelet model
1. Introduction

Clean energy generation processes are a crucial consideration in the design of modern thermal energy power units as combustion of fossil fuels continues to cause serious issues for the environment and the geopolitical climate of the world. Secure supplies of energy and chemical/combustion products are keystones not only of society but also of our industries. However, energy use has consequences that extend beyond immediate applications. Environmental impacts can be particularly significant in the case of fossil fuel combustion as this process contributes significantly to the emissions of nitric oxide, carbon monoxide and carbon dioxide ($\text{NO}_x, \text{CO}, \text{CO}_2$) and unburned hydrocarbons. A prominent example for improvement is the reduction of greenhouse gas emissions during combustion, which still provides more than 80% of the energy supply worldwide. Saving of limited resources and reduced environmental impact by unwanted by-products are the driving force for intense research in combusting flows. Sixty years ago exhaust emissions such as $\text{NO}_x, \text{CO}$ and smoke were not a consideration, while now they need to meet strict emission regulations which are expected to become more stringent with time [1-4].

Clean energy and alternative energy have become major areas of research worldwide for sustainable energy development. Among the important research and development areas are hydrogen and synthesis gas (syngas) usage for electricity generation and transport technology [5]. Most of the world’s current supply of hydrogen is derived from fossil fuels and therefore development of clean energy technology would allow continued use of fossil fuels such as coal without substantial emissions of greenhouse gases such as $\text{CO}_2$ [6-7]. It can also balance the energy between supply and demand, a strategic and necessary choice for realising the coordinated development of energy, environment and economy [8]. In order to properly
understand the effects of adding hydrogen to enrich hydrocarbon combustion it is important to understand the characteristics of combustion processes for syngas mixtures. Therefore ongoing development of hydrogen and syngas combustion technology as an appropriate type of future energy source is playing an increasingly important role in the clean energy strategy.

It is well established in the literature that hydrogen and syngas production from fossil fuel such as coal can have significant influence on modern day clean energy generation, particularly application of electricity such as integrated gasification combined cycle (IGCC) including possible treatment for CO₂ capture. Recently studies have shown substantial interest on IGCC technology to employ hydrogen and syngas fuels for the gas turbine combustion [9-10]. This integration of energy conversion processes provides more complete utilization of energy resources, offering high efficiencies and ultra-low pollution levels [11]. Ultimately IGCC systems will be capable of reaching efficiencies of 60% with near-zero pollution. The unique advantages of IGCC systems have led to potential applications of gasification technologies in industry because gasification is the only technology that offers both upstream (feedstock flexibility) and downstream (product flexibility) advantages. A series of important laboratory scale experimental investigations on syngas combustion are reported in the literature, including studies of the scalar structure of CO/H₂/N₂ nonpremixed flames [12], laminar flame speeds of H₂/CO/CO₂ premixed flames [13], effects of nitrogen dilution on flame stability of syngas mixtures [14], and global turbulent consumption speed of syngas H₂/CO mixtures [15].

Non-premixed (or diffusion) combustion occurs in many thermal energy applications where fuel and oxidizer are not perfectly premixed before entering the combustion chamber. Because many practical combustion devices operate with non-premixed flames in the
presence of turbulent flow, investigation of the characteristics of syngas non-premixed turbulent combustion has become important in order to gain a better understanding of modern combustion systems for clean combustion. In recent decades, computational combustion has made remarkable advances due to its ability to deal with a wide range of scales, complexity and almost unlimited access to data [16]. Large eddy simulation (LES) in which large scales are resolved and small scales are modelled, is evolving as an extremely valuable computational tool from which much can be learned [17]. In the simulation of turbulent combustion, the unsteady three-dimensional (3D) nature of LES has many advantages for turbulence modelling over the classical Reynolds-averaged Navier-Stokes (RANS) approach. However, since chemical reactions occur well below the resolution limit of the LES filter width, the technique requires a separate modelling strategy to predict the combustion characteristics. Several groups have employed the LES technique and different combustion models to simulate turbulent non-premixed flames which include equilibrium chemistry [18-20], steady laminar flamelet model [21-22], unsteady laminar flamelet model [23], flamelet-progress variable approach [24], conditional moment closure model [25], linear eddy mixing combustion model [26] and probability density function approach [27]. Nevertheless, there is a lack of knowledge on the general suitability of these models. In this context, experimental validation can play a significant role in assessing the model performance.

A detailed analysis of fuel variability and flame structures of syngas mixtures is of fundamental importance. However, the majority of modelling investigations reported above focused on modelling aspects and validation, and did not provide sufficient details about flame characteristics with respect to variable syngas fuel mixtures. The objective of the present work is to perform LES for four different syngas non-premixed fuel mixtures and extract information from the numerical databases to analyse the effects of fuel variability and
flame characteristics in the context of non-premixed syngas combustion. For this, a well established laboratory scale non-premixed turbulent jet flame configuration which burns a fuel mixture of 75% of H₂ and 25% of N₂ is selected as a base case [28]. Four different syngas mixtures of H₂/N₂ and H₂/CO have been considered for a similar jet flame configuration with identical conditions except for changing fuel compositions, to enable the extraction of information with respect to fuel variability. For a better understanding, extensive analyses has been executed to uncover the origin of the found deviations. This is a continuation of our previous work in which we focused on low Reynolds number direct numerical simulation (DNS) of hydrogen non-premixed combustion [29]. The paper is organised as follows. Section 2 presents the governing equations and modelling followed by the details of numerical methods in section 3. Section 4 discusses simulated test cases followed by the results and discussion conclusion in section 5. Finally, conclusions from the study are drawn in section 6.

2. Governing Equations and Modelling

2.1. LES governing equations

LES is based on the premise that the large eddies of the flow are dependent on the flow geometry, making them highly anisotropic, whilst the smaller eddies are self similar and have a universal character, or are close to isotropy. In LES, the large scale motions of the flow are calculated exactly, whilst the effect of the smaller universal scales (so called sub-grid scales) are modelled using a sub-grid scale (SGS) model. A spatial filter is generally applied to separate the large and small scale structures. For a given function \( f(x,t) \) the filtered field \( \overline{f(x,t)} \) is determined by convolution with the filter function \( G \)
\[ f(x) = \int_{\Omega} f(x') G(x-x', \Delta(x)) dx', \]  

(1)

where the integration is carried out over the entire flow domain \( \Omega \) and \( \Delta \) is the filter width, which varies with position. A number of filters are used in LES such as top hat or box filter, Gaussian filter, spectral filter. In the present work, implicit filtering by the numerical discretisation is used. This is approximately equivalent to a top-hat filter having a filter-width \( \Delta_j \) proportional to the size of the local cell. In turbulent reacting flows large density variations occur. These are treated using Favre filtered variables, which leads to the transport equations for Favre filtered mass, momentum and mixture fraction:

\[ \frac{\partial \ Fluid}{\partial t} + \frac{\partial \ Fluid_{\cdot x_j}}{\partial x_j} = 0 \]  

(2)

\[ \frac{\partial \ Fluid_{\cdot x_i}}{\partial t} + \frac{\partial (Fluid_{\cdot x_i} u_j)}{\partial x_j} = -\frac{\partial \ Fluid_{\cdot x_i}}{\partial x_i} + \frac{1}{2} 2 \rho (\nu + \nu_t) \left( \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) - \frac{1}{3} \delta_i^j \frac{\partial u_k}{\partial x_i} \right] 
+ \frac{1}{3} \frac{\partial}{\partial x_j} \left[ \rho \delta_i^j \tau_{kk} \right] + \rho g_i \]  

(3)

\[ \frac{\partial \ Fluid}{\partial t} + \frac{\partial (\ Fluid_{\cdot x_j} \ Fluid_{\cdot x_j})}{\partial x_j} = \frac{1}{\delta x_j} \left[ \ Fluid_{\cdot x_j} \left( \ Fluid_{\cdot x_j} \ Fluid_{\cdot x_j} \right) \right] \]  

(4)

In the above equations \( \rho \) represents the density, \( u_i \) is the velocity component in \( x_i \) direction, \( p \) is the pressure, \( \nu \) is the kinematic viscosity, \( f \) is the mixture fraction, \( \nu_t \) is the turbulent viscosity, \( \sigma \) is the laminar Schmidt number, \( \sigma_t \) is the turbulent Schmidt number and \( \tau_{kk} \) is the isotropic part of the sub-grid scale stress tensor. An over-bar describes the application of the spatial filter while the tilde denotes Favre filtered quantities. The laminar Schmidt number was set to 0.7 and the turbulent Schmidt number for mixture fraction was set to 0.4. Finally to
close these equations, the turbulent eddy viscosity \( \nu_t \) in Eq. (3) and (4) has to be evaluated using a model equation.

### 2.2. Modelling of turbulent eddy viscosity

In this work, the turbulent eddy viscosity \( \nu_t \) is calculated using the Smagorinsky eddy viscosity model. The Smagorinsky eddy viscosity model [30] uses a model parameter \( C_s \), the filter width \( \bar{\Delta} \) and strain rate tensor \( S_{i,j} \) such that

\[
\nu_t = C_s \bar{\Delta}^2 |S_{i,j}| = C_s \bar{\Delta}^2 \left| \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right|
\]

The model coefficient \( C_s \) is evaluated using the dynamic procedure which calculates the model coefficient dynamically using instantaneous local flow conditions. This dynamic procedure involves the application of two spatial filters and the model coefficient is computed dynamically as the calculation progresses (rather than being imposed a priori) based on the energy content of the smallest resolved scale. In addition to the grid filter, which separates the resolved and sub-grid scales, a test filter is used, whose width \( \Delta \) is larger than the grid filter width \( \bar{\Delta} \). Similar to grid scale filter, the test scale filter also defines a new set of stresses leading to a test level sub-grid scale tensor

\[
T_{ij} = \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j
\]

The resolved turbulent stresses or Leonard stresses

\[
L_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j
\]
which represent the contribution of the smallest resolved scales to the Reynolds stresses, can be computed from the resolved velocity, and are related to the sub-grid scale stresses, $\tau_{ij}$ by the identity of Germano et al. [31]

\[ L_{ij} = T_{ij} - \hat{\tau}_{ij} \]  

(8)

The sub-grid and sub-test scale stresses are then parameterised using the eddy viscosity approach

\[ \tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2C\Delta^2 \left[ \tilde{S} \right] \tilde{S}_{ij} = -2C\beta_{ij} \]  

(9)

\[ T_{ij} - \frac{\delta_{ij}}{3} T_{kk} = -2C\Delta^2 \left[ \tilde{S} \right] \tilde{S}_{ij} = -2C\alpha_{ij} \]  

(10)

Substituting equations (9) and (10) into (8) yields

\[ L_{ij}^a = L_{ij} - \frac{\delta_{ij}}{3} L_{kk} = -2C\alpha_{ij} + 2C\beta_{ij} \]  

(11)

This is a set of five independent equations. To obtain a single coefficient from the five independent equations, Lilly [32] proposed to minimise the sum of the squares of the residual:

\[ E_{ij} = L_{ij}^a + 2C\alpha_{ij} - 2C\beta_{ij} \]  

(12)

By contracting both sides (11) with $\alpha_{ij} - \beta_{ij}$ to yields

\[ C(x,t) = -\frac{1}{2} \frac{L_{ij}^a(\alpha_{ij} - \beta_{ij})}{(\alpha_{nn} - \beta_{nn})(\alpha_{nn} - \beta_{nn})} \]  

(13)

The Smagorinsky coefficient $C_s$ can be computed as $C_s = \sqrt{C}$.

However, Germano et al. [31] dynamic procedure involves the production of local negative eddy viscosity values which need further treatments. To avoid this difficulty, here we employed a less expensive localised dynamic procedure proposed by Piomelli and Liu [33],
which involves finding an approximate solution to the integral equation by using the value of constant $C$ at previous time step.

### 2.3. Modelling of combustion

Modelling of non-premixed combustion applications often requires the use of detailed chemistry models in two and three dimensional simulations. In order to account for the combustion chemistry, a modelling approach is required to capture the chemical reactions occurring at the sub-grid scale. Modelling of combustion applications frequently involves the use of detailed chemistry models including many chemical species and reactions. The laminar flamelet approach plays an important role in both laminar and turbulent combustion modelling [34]. Here we employed the steady laminar flamelet model which generates flamelets by solving one-dimensional flamelet equations for a laminar counter-flow configuration. The flamelet calculations were performed using the Flamemaster code developed by Pitsch [35], which incorporates the GRI 2.11 mechanism with detailed chemistry [36-37]. An assumed probability density function (PDF) for the mixture fraction is chosen as a means of modelling the sub-grid scale mixing with a $\beta$ PDF used for the mixture fraction. Two key variables known as mixture fraction and scalar dissipation rate determine the thermochemical composition of the turbulent flame. The variables such as density, temperature and species concentrations depend on Favre filtered mixture fraction, mixture fraction variance and scalar dissipation rate. The joint probability density function (PDF) $P(f, \chi)$ of mixture fraction $f$ and scalar dissipation rate $\chi$ is used to determine the filtered values of temperature, density and species mass fractions. Thus the filtered value of the scalar variable is given by
In the flamelet model, it is assumed that the mixture fraction and the scalar dissipation rate are statistically independent. Thus the joint PDF can be decomposed into two parts such that

$$
\phi = \int_0^1 \int_0^1 \phi(f, \chi) P(f, \chi) df d\chi
$$

(14)

Here we use an assumed ($\beta$) probability density function (PDF) for the mixture fraction as a means of modelling the sub-grid scale mixing. The two independent PDFs can be written as

$$
P(f) = \frac{\Gamma(\beta_1 + \beta_2)}{\Gamma(\beta_1)\Gamma(\beta_2)} f^{\beta_1-1}(1-f)^{\beta_2-1}
$$

(16)

$$
P(\chi) = \frac{1}{\chi \sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2} (\ln(\chi) - \mu)^2\right)
$$

(17)

where

$$
\beta_1 = f \left[ \frac{f(1-f)}{f^2} - 1 \right]
$$

$$
\beta_2 = \frac{(1-f)}{f} \beta_1
$$

However the filtered mixture fraction variance $f^2$ and filtered scalar dissipation rate $\chi$ still remain unknown quantities which need to be modelled. The mixture fraction variance and the scalar dissipation rate are modelled using the model equations:

$$
f^2 = C \Delta^2 \left( \frac{\partial f}{\partial x_j} \frac{\partial f}{\partial x_j} \right)
$$

(18)
\[ \chi = 2 \left( \frac{v}{\sigma} + \frac{v}{\sigma_j} \right) \left( \frac{\partial f}{\partial x_j} \frac{\partial f}{\partial x_j} \right) \]  

(19)

where \( C \approx 0.1 \) has proved successful and \( \bar{\Delta} = (\bar{\Delta}, \bar{\Delta}, \bar{\Delta}) \).

3. Numerical methods

The set of equations noted above are solved by the large eddy simulation code PUFFIN originally developed by Kirkpatrick et al. [38-39] and later extended by Ranga Dinesh et al. [40-41]. PUFFIN computes the temporal development of large-scale flow structures by solving the transport equations for the Favre-filtered continuity, momentum and mixture fraction. The equations are discretised in space with the finite volume formulation using Cartesian coordinates on a non-uniform staggered grid. Second order central differences (CDS) are used for the spatial discretisation of all terms in both the momentum equation and the pressure correction equation. This minimizes the projection error and ensures convergence in conjunction with an iterative solver. The diffusion terms of the scalar transport equation are also discretised using the second order CDS. However, discretisation of convection term in the mixture fraction transport equation using CDS would cause numerical wiggles in the mixture fraction. To avoid this problem, here we employed a Simple High Accuracy Resolution Program (SHARP) developed by Leonard [42].

In the LES code, an iterative time advancement scheme is used to advance a variable density calculation. First, the time derivative of the mixture fraction is approximated using the Crank-Nicolson scheme. The flamelet library yields the density and calculates the filtered density field at the end of the time step. The new density at this time step is then used to advance the momentum equations. The momentum equations are integrated in time using a second order
hybrid scheme. Advection terms are calculated explicitly using second order Adams-Bashforth while diffusion terms are calculated implicitly using second order Adams-Moulton to yield an approximate solution for the velocity field. Finally, mass conservation is enforced through a pressure correction step. Typically 8-10 outer iterations of this procedure are required to obtain satisfactory convergence at each time step. The time step is varied to ensure that the Courant number $C_o = \Delta tu_i/\Delta x_i$ remains approximately constant where $\Delta x_i$ is the cell width, $\Delta t$ is the time step and $u_i$ is the velocity component in the $x_i$ direction. The solution is advanced with a time step corresponding to a Courant number in the range of $C_o = 0.3$ to 0.6. The Bi-Conjugate Gradient Stabilized (BiCGStab) method with a Modified Strongly Implicit (MSI) preconditioner is used to solve the system of algebraic equations resulting from the discretisation.

Simulations for all four flames were carried out with the dimensions of 600×200×200mm in the x (axial direction), y and z directions respectively and employed a non-uniform Cartesian grid with 200×130×130 (approximately 3.4 million) cells. The mean axial velocity distribution for the fuel inlet is specified using a power law profile and turbulent fluctuations is generated from a Gaussian random number generator, which is then added to the mean axial profile such that the inflow has the same turbulence kinetic energy levels as those obtained from the experimental data [28]. A top hat profile is used as the inflow condition for the mixture fraction. All computations were carried out for a total time of 0.27s – enough to ensure that the solution has achieved a sufficient number of flow passes to provide good statistical data. Fig. 1 shows the three-dimensional (3D) geometry of the jet flame considered here (showing an iso-surface of the unsteady axial velocity of $u=10$ m/s obtained from the LES) and the dimensions of the computational box including boundary conditions used.
4. Simulated test cases

In the current investigation, four different syngas flames – two for H₂/N₂ and another two for H₂/CO fuel mixtures – have been considered. The flow conditions and fuel mixtures for all four flames are outlined in Table 1. Considering the fuel composition, four flames have been named as flame HN1 (75% H₂ and 25% N₂), flame HN2 (50% H₂ and 50% N₂), flame HCO1 (70% H₂ and 30% CO) and HCO2 (30% H₂ and 70% CO). The base flame HN1 has been selected to correspond with a well-established experimental data archive [28], and the fuel mixtures of other three flames HN2, HCO1 and HCO2 have been selected to investigate the fundamental flame properties of important syngas fuel mixtures of H₂-rich, H₂-lean and CO-rich, CO-lean flames. The configuration of all four flames consists of a D=8mm diameter fuel jet with a jet velocity of 42.3 m/s resulting in a Reynolds number of 9,300.

5. Results and discussion

LES of flames corresponding to four different syngas fuel mixtures named as flames HN1, HN2, HCO1 and HCO2 varying from H₂-rich to H₂-lean and CO-rich to CO-lean including N₂ have been performed. These compositions were chosen to cover potentially important syngas mixture variations. The flame characteristics including temperature and chemical compositions (major species) of the syngas non-premixed flames are provided here to illustrate the effects of fuel variability on the flame structures. The results focus on both temporal characteristics and time-averaged comparisons to obtain a good understanding of flame structures in the context of turbulent non-premixed syngas combustion. The results are discussed in two sub-sections: instantaneous flame structures and time-averaged flame
structures. The focus of the discussion is on the effects of fuel variability on both instantaneous and time-averaged flame structures of syngas mixtures once the flame is fully developed.

5.1 Instantaneous flame structures

Fig. 2 displays instantaneous 3D iso-surfaces of flame temperature at various values from T=500K to the maximum flame temperature at time t=0.2s for the corresponding syngas fuel mixture. The effects of turbulence is clearly apparent in the topology of the 3D flames. Within a turbulent flow, the diffusion flame is continuously distorted and stretched by velocity fluctuations inducing inhomogeneities in the mixing of the reactants, which is clearly apparent from the 3D flame structures for all four syngas flames. One aspect of the spreading of the temperature field corresponds to the transient response induced by the turbulent mixing, which modifies the instantaneous temperature and chemical species and therefore the chemical activity. The other aspect is the fuel variability which significantly modifies the flame vortex structure and temperature values as a result of corresponding chemical and transport properties. Particularly, the H$_2$-rich and N$_2$-lean flame HN1 display different vortical structures compare to the 50% H$_2$/ 50% N$_2$-fueled HN2 flame. Comparisons between HN1 and HN2 clearly demonstrate how the inert gas N$_2$ affects the flame structure of the H$_2$-rich non-premixed flame. The addition of N$_2$ to H$_2$ tends to lower the flame temperature but increase the formation of vortical structures which eventually affects the diffusion process compare to H$_2$-rich and N$_2$-lean flame. While variation in the H$_2$/N$_2$ ratio largely affects the flame dynamics including the flame temperature values, the ratio of H$_2$/CO seems to have a little effect on flame temperature but a large impact on formation of
vortical structures and flame thickness. In Fig. 2, it can be seen that H₂-rich and CO-lean flame HCO1 displays much larger and thicker pockets of maximum flame temperature (T=2200K), while H₂-lean and CO-rich flame HCO2 exhibits smaller and thin pockets of maximum flame temperature (again T=2200K). In generally, instantaneous results in Fig. 2 demonstrate the influence of H₂, N₂ and CO on flame temperature and flame thickness including small wrinkles of simulated non-premixed syngas flames.

Instantaneous two-dimensional streamwise and cross-streamwise contour plots of mixture fraction and flame temperature at time t=0.2s are shown in Fig. 3. Both streamwise and cross-streamwise instantaneous mixture fraction distributions between H₂-rich flame HN1 and equally fueled H₂/N₂ flame HN2 display slight differences, but the differences are wider between flames of H₂-rich flame HCO1 and CO-rich flame HCO2. Although the upstream distribution exhibits similar behaviour for all four flames, the downstream movement is significantly affected with respect to fuel variability particularly for the H₂-rich and CO-lean flame HCO1 compared to H₂-lean and CO-rich flame HCO2. This could be because of the differences in diffusivity associated with the amount of hydrogen available in the fuel. As expected, the streamwise and cross-streamwise temperature distributions display large differences between all four flames. The H₂-rich flame HN1 exhibits large pockets of high temperature compare to HN2 which supply equal amount of H₂ and N₂. Both H₂/CO based HCO1 and HCO2 show large area of high temperature in the downstream region compared to the two H₂/N₂ based flames. However, the H₂-rich and CO-lean flame HCO1 clearly demonstrates a much greater flame thickness downstream compare to all other three flames. It can be seen that the variations of transport properties and chemistry associated with fuel variability can change the mixing rate and accordingly the chemical heat release and
temperature distributions. Having discussed the instantaneous structures of all four syngas flames the analysis now focuses on the time-averaged statistics.

5.2 Time-averaged flame structures

Time-averaged statistics were obtained by averaging the flame quantities after the initial stage of the simulation. Fig. 4 shows the contour plots of time averaged mean temperature for flames HN1, HN2, HCO1 and HCO2 respectively. All four flames show similar behaviour in the near nozzle region, but start to deviate at the far field. Particularly, the maximum mean temperature structures in the downstream centreline region differ significantly with fuel variability.

Radial profiles of time-averaged mean mixture fraction and mixture fraction variance are shown in Figs. 5 and 6. It is evident that the radial spread of the mean mixture fraction is in good agreement with the experimental measurements, but under predicted at further downstream for its variance. This is may be due to numerical diffusion associated with the SHARP advection scheme. This is difficult to avoid, since using a non-dissipative advection scheme would lead to unphysical values of mixture fraction. Overall predictions of mixture and its variance, however, show reasonably good agreement at all locations for the H$_2$-rich HN1 flame. As seen in Fig.5 (b), adding N$_2$ does slightly affects the centreline value of mean mixture fraction particularly at downstream (x=320mm), but largely follow a similar shape distribution for the mixture fraction variance. Again, the mixture fraction of H$_2$-rich and CO-lean flame HCO1 follows a similar shape distribution and values as HN1, but exhibits different distribution for H$_2$-lean and CO-rich flame HCO2. This behaviour is also apparent for the mixture fraction variance.
Fig. 7 shows radial profiles of mean temperature at different downstream axial locations for all four syngas flames. In Fig. 7, it can be seen that the mean temperature is slightly underpredicted at x=80, 160mm and 320mm for H₂-rich flame HN1, which might be the result of the discrepancy of the calculated radial spread of the mean mixture fraction and mixture fraction compared to the experimental measurements. There might be other aspects which also cause small discrepancy between calculated results and experimental data such as the diffusion based molecular mixing rate and heat release may not have been well modelled. The flame may be subject to different shear effects associated with the fuel variability, while the selected flamelet's with thermo-chemical properties extracted from the corresponding strain rates may not be accurate enough. However, given the large density gradient between H₂ and air, the comparison of the calculated temperature field with experimental data for flame HN1 is reasonable at the considered axial locations. In a steady diffusion flame, the heat loss by diffusion and convection is balanced by the heat release in the reaction zone. For the equally fueled HN2 flame, the peak flame temperature is much lower than that of the H₂-rich and N₂-lean HN1 flame. The high temperature in flame HN1 is mainly the result of the high level of diffusivity and reactivity of H₂. However both the H₂-rich and CO-lean flame HCO1 and H₂-lean and CO-rich flame HCO2 display different mean temperature distributions particularly at the downstream region compared to the H₂-rich and N₂-lean HN1 flame. Both the H₂-rich flame HCO1 and CO-rich flame HCO2 show similar maximum mean temperature. This might occur as a result of the higher molar heating value of CO, which tends to increase the flame temperature. However, more importantly radial profiles of H₂-rich flame HCO1 exhibits high temperature for far radial locations compared to CO-rich flame HCO2, which confirms the occurrence of a greater flame thickness for the H₂-rich H₂/CO mixture compared to the CO-rich H₂/CO mixture. Depending on high
hydrogen or high carbon monoxide, the diffusivity level changes from one flame to another and thus leads to different heat release patterns. The temperature results of all four flames suggest that fuel variability plays a key role in determining the local flame temperature including flame thickness, both unsteadily and steadily.

The next parameters of interest are the combustion products. Figs. 8 and 9 show the mass fractions of H₂ and H₂O. The comparisons between LES results and experimental data are reasonable for both mass fractions of H₂ and H₂O. The trends of mass fractions of H₂ are consistent with the mixture fraction while mass fractions of H₂O are consistent with those of temperature showing different peak values for all four flames. The highest values of H₂ and H₂O mass fractions are gradually decreasing for HN2 and HCO2 with the lower amount of H₂ availability in the syngas fuel mixture. Since both HCO1 and HCO2 contain a sufficient percent of CO, Fig. 10 shows the time-averaged radial profiles of CO and CO₂ at different downstream axial locations. It can be seen that the addition of CO in the fuel leads to both unburnt CO and burnt CO₂ in the combustion products. Compared to H₂-rich but CO-lean flame HCO1, H₂-lean but CO-rich flame HCO2 show higher mass fractions of CO and CO₂ as a result of high CO concentration in the inlet fuel syngas mixture. In all considered syngas flames, the steady laminar flamelet model appear to be sufficient to provide accurate predictions for the flame temperature and major species. However, quantifying the radical minor species such as hydroxyl (OH) and nitric-oxide (NOₓ) are more difficult in the steady flamelet framework. One possibility is to employ an unsteady flamelet model which would potentially quantify the NOₓ and radical species more accurately.
6. Conclusions

The primary focus of this work was to examine the effects of fuel variability on flame characteristics of turbulent non-premixed syngas combustion using large eddy simulations. Four different syngas mixtures including two using $\text{H}_2/\text{N}_2$ and another two using $\text{H}_2/\text{CO}$ have been considered. The fuel variability effects have been investigated by examining both the instantaneous flame structures and time-averaged flame properties.

It has been found that diffusivity of hydrogen dominates the flame characteristics and combustion dynamics of $\text{H}_2$-rich combustion. Particularly, higher diffusivity in the $\text{H}_2$-rich fuels leads to formation of a thicker flame than that found for the CO-rich fuels. While the $\text{H}_2/\text{CO}$ ratio has a minor influence on flame temperature, it plays a major role in flame thickness, strain rate and thus flame stability. The flame structure and maximum flame temperature largely depend on the syngas fuel compositions. Due to the high reactivity and diffusivity of $\text{H}_2$, the flame structures of syngas flames are highly likely to be different than that of traditional natural gas flames. Further extraction of the quantities such as flammability limits, stretch sensitivity and extinction strain rate could permit us to quantitatively estimate the involvement of individual fuel properties in the complete momentum exchange, heat release and their impact on other aspects such as radiative energy transfer and radical combustion products of syngas flames for future clean combustion systems.

Acknowledgement

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References


Table captions

Table 1. Flame conditions and compositions of the syngas fuels

Figure Captions

Fig.1. Geometry of the turbulent non-premixed jet flame with a diameter of D=8mm and inlet jet velocity of $U=42.3$ m/s (generated for the velocity iso-values of $u=10$ m/s at time $t=0.2s$)

Fig.2. Instantaneous three-dimensional iso-surfaces with iso-values (1) 700K, (2) 1000K, (3) 1500K, (4) maximum values ((a4) 2100K, (b4) 1800K (c4,d4) 2200K) of the flame temperature of flames (a) HN1 (b) HN2 (c) HCO1 and (d) HCO2 at time $t=0.2s$

Fig.3. Instantaneous two-dimensional streamwise contour plots of mixture fraction (a1) HN1, (b1) HN2, (c1) HCO1, (d1) HCO2, flame temperature (a2) HN1, (b2) HN2, (c2) HCO1, (d2) HCO2 and two-dimensional cross-streamwise contour plots of mixture fraction (a3) HN1, (b3) HN2, (c3) HCO1, (d3) HCO2 and flame temperature (a4) HN1, (b4) HN2, (c4) HCO1 and (d4) HCO2 at axial location $x=320$mm at time $t=0.2s$.

Fig.4. Time-averaged two-dimensional contour plots of mean temperature for flames (a) HN1, (b) HN2, (c) HCO1 and (d) HCO2.

Fig.5. Time-averaged mean mixture fraction for flames (a) HN1, (b) HN2, (c) HCO1 and (d) HCO2. Lines denote LES data and symbols denote experimental data.

Fig.6. Time-averaged mixture fraction variance for flames (a) HN1, (b) HN2, (c) HCO1 and (d) HCO2. Lines denote LES data and symbols denote experimental data.

Fig.7. Time-averaged mean temperature for flames (a) HN1, (b) HN2, (c) HCO1 and (d) HCO2. Lines denote LES data and symbols denote experimental data.
Fig. 8. Time-averaged mass fraction of $\text{H}_2$ for flames (a) HN1, (b) HN2, (c) HCO1 and (d) HCO2. Lines denote LES data and symbols denote experimental data.

Fig. 9. Time-averaged mass fraction of $\text{H}_2\text{O}$ for flames (a) HN1, (b) HN2, (c) HCO1 and (d) HCO2. Lines denote LES data and symbols denote experimental data.

Fig. 10. Time-averaged mass fraction of CO for flames (a) HCO1, (b) HCO2 and CO$_2$ for flames (c) HCO1, (d) HCO2. Lines denote LES data
Tables

Table 1. Flame conditions and compositions of the syngas fuels

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<td>CO%</td>
<td>0</td>
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</table>
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