Flashback Analysis for Hydrogen/Methane mixtures for Premixed Swirl Combustion

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ABSTRACT

The flashback problem which occurs by using lean premixed combustion in gas turbines is considered. Flashback simulation studies using CFD modelling package are performed for a wide range of hydrogen/methane (H\textsubscript{2}/CH\textsubscript{4}) blends combusted by air using a swirl burner under premixed conditions. The laminar flame speed was calculated for H\textsubscript{2}/CH\textsubscript{4} blends from pure methane up to pure hydrogen at various pressures, temperatures and equivalence ratios. This was done by using CHEMKIN-PRO software package with PREMIX code and an algebraic expression derived by asymptotic methods incorporated with Le Chatelier’s Rule-like correlation. The feasibility of using a new approximation for laminar flame speed of H\textsubscript{2}/CH\textsubscript{4} blends based on the gravimetric mixture ratio was checked and compared with the previous calculations. The new approximation gave a good prediction at various conditions. The numerical values for laminar flame speed calculated by CHEMKIN are then fed to FLUENT CFD model to create a PDF table for turbulent premixed combustion calculations and flashback studies. Flashback limits were defined and determined for H\textsubscript{2}/CH\textsubscript{4} blends ranging from 0% (pure methane) up to 100% (pure hydrogen) based on the volumetric composition at atmospheric pressure and 300K for various equivalence ratios. The results show that the use of up to 50% blends of methane and hydrogen causes fewer problems with flame stability and flashback compared with the use of pure hydrogen. Also, the flashback limits depend on the values for both laminar and turbulent flame speed. What emerges is the need for more theoretical and experimental research work to obtain more accurate values for flame speeds.

Introduction

Hydrogen (H\textsubscript{2}) can be considered to be one of the most promising clean alternative fuels. However the high cost of producing pure hydrogen and its high flame speed restrict its commercial usage. Instead of using pure hydrogen, hydrogen-methane (H\textsubscript{2}/CH\textsubscript{4}) blends are receiving attention as alternative fuels for power generation applications for three reasons. The first is related to the opportunity of adding H\textsubscript{2} to natural gas in order to improve performance and reduce CO\textsubscript{2} emissions. The second is due to concern about global warming and prospect of using hydrogen in both fuel cells and combustion devices. The third is to enhance the utilization of gasified biomass and other by-product gases derived from some industrial processes in the form of producer gases containing mainly H\textsubscript{2} and CO which can also be blended with methane [1, 2].

Another way to reduce pollutant emissions, particularly NOx emissions is to operate with lean premixed combustion. Lean premixed (LP) gas turbine combustion has considerable advantages in terms of allowing lower overall flame temperatures, whilst smearing the flame and combustion processes over larger volumes. However, the gains made by LP operating conditions can be accompanied by stability problems. Premixed flames are naturally more susceptible to static and dynamic instability due to a lack of inherent damping mechanisms [3, 4]. Swirl burners can be used to stabilize the flame. Swirl flows have been studied for decades, with detailed descriptions in the work of Syred [5, 6] and Gupta et al. [7]. Other authors like Vanoverberghe [8] and Coghe et al. [9] have demonstrated the reduction of emissions by increasing swirl, producing flames stabilized by the surrounding structures, such as inner and outer recirculation zones, formed as a consequence of the dynamics of the swirling flow.
mechanism. However, the structures that drive these systems are only inferred in these studies or studied partially, without fundamental knowledge of their interaction and co-existence. Huang et al. [10-12] studied the effect of inlet swirl on the flow development and combustion dynamics in lean premixed swirl-stabilized combustor. They found that when the inlet swirl number exceeds a critical value, a vortex-breakdown-induced central toroidal swirl-stabilized combustor. They found that when the inlet swirl number exceeds a critical value, a vortex-breakdown-induced central toroidal recirculation zone is established in the downstream region. As the swirl number increases further, the recirculation zone moves upstream and merges with the wake recirculation zone behind the centerbody. Excessive swirl may cause the central recirculating flow to penetrate into the inlet annulus and lead to the occurrence of flame flashback.

Flashback occurs when the gas velocity becomes smaller than the burning velocity and the flame propagates upstream into the premixer passages. Since these passages cannot withstand high temperatures, hence hardware damage occurs [13-15]. Flashback is also a concern as the central recirculation zone can extend back around the fuel injector to the burner backplate, thus increasing the risk of flashback [7-9, 16]. If the Central Recirculation Zone (CRZ) does extend back to the injector, this can leave thick layers of carbonaceous deposit on the injector surfaces, reducing the efficiency and increasing maintenance requirements. Flashback is an important issue in lean premixed combustion systems that use hydrogen as an additive fuel due to the widely varying flame speeds of the mixtures considered. As such, the effect of fuel composition variation upon flashback depends upon the corresponding change in local flame speed, both laminar and turbulent [17]. Generally, flashback can be initiated by the four following causes, [18-21]:

- Flame propagation in the boundary layer,
- Turbulent flame propagation in the core flow,
- Violent combustion instabilities, and
- Combustion induced vortex breakdown (CIVB).

In swirling flows, in particular, several potential modes of flashback can occur [19, 20, 22]. The first mode is that of flashback in the boundary layer due to the low velocities. The second mode refers to flashback in the core flow. The two modes take place when local burning velocity exceeds the flow velocity, allowing the flame to propagate upstream into the premixer passages. In some cases, flashback can occur even though the local flame velocity is less than the flow velocity. The flame can cause the vortex upstream to breakdown and this creates a negative flow region to form ahead of it (due to adverse pressure gradients) which causes it to advance further upstream. This phenomenon is referred to “combustion induced vortex breakdown” [22] and is caused by the temperature ratio across the flame [23]. Lieuwen et al. concluded further that “combustion induced vortex breakdown” is not influenced by the chemical kinetic characteristics of the mixture [24]. Furthermore, Noble and coworkers related this phenomenon to the pressure rise upstream of the flame due to the divergence of the upstream flow caused by the inclined flame front [25]. In general, flashback is greatly influenced by the variations in fuel composition that affect the combustion properties of the mixture, notably, the local burning velocity [26].

The laminar flame speed is an important property when studying combustion modelling especially turbulent combustion and flashback. During the last decades significant progress is achieved in the understanding of methane as well as hydrogen flames. While the combustion characteristics of pure mixtures of methane-air and hydrogen-air have been extensively studied over the years, the knowledge regarding the combustion of mixtures containing both methane and hydrogen is limited [27]. Experimental data available in literature are often determined at ambient conditions. In gas turbines however conditions are different as they work under high pressure and temperature. The experimental [27-31] and numerical results [32-34] show an increase of the burning velocities as a result of hydrogen addition to methane. All results show that hydrogen enhance the combustion characteristics of methane.
In this paper, the modelling of swirl lean premixed combustion is discussed. Firstly, the laminar flame speed of H₂/CH₄ blends is calculated by CHEMKIN software with PREMIX package. The values are compared with an algebraic expression derived by asymptotic methods incorporated with Le Chatelier’s Rule-like correlation. Then a new approximation for calculating the laminar flame speed of H₂/CH₄ mixtures is suggested and compared with the previous calculations. Secondly, FLUENT software is used to simulate the combustion of pure methane and H₂/CH₄ blends in a high pressure gas turbine combustor. The effect of the blend ratio on the flame stability is studied. Also the flashback limits of H₂/CH₄ combustion are determined from pure methane up to pure hydrogen and combinations between.

**Physical Model**

The physical model considered consists of a single swirler injector and an axi-symmetric chamber. The combustor is a High Pressure Optical Combustor (HPOC) Test Module that has been designed for use on the High Pressure Combustor Rig (HPCR) and consists of a pressure casing and optical combustor which is shown in figure 1. The HPOC has the flexibility to run liquid and gaseous fuels and the burner consists of a premixed main with diffuse CH₄ pilot. The fuel/air mixture is assumed to be perfectly premixed before entering the combustor. The combustion chamber consists of two jointed parts. The first part is the optical section while the other is the non-optical part. Both parts have the same shape and dimensions. Both cross sections are square with chamfered edges to allow good optical access for combustion diagnostics. Each is (152 x 152 mm) cross section and 208 mm long. All edges are chamfered at 24 mm at each corner.

![Figure 1: High Pressure Optical Combustor](image-url)

The rigs can be fired with variable quality gaseous and liquid fuels and are supplied by a range of heavy-duty industrial components and control systems, including a compressor, large-scale heat exchanger, high-specification pipe-work with a dedicated control room. The combustion facility operating range for the optical combustor are:

- **Air flow rate**: < 5 kg/s
- **Absolute Pressure**: < 16 bar
- **Temperature**: < 900 K

The realistic working section operating condition are up to ~2.5 kg/s air through the combustor head at 15 bar and 875K. The flexible premixed burners for HPOC are:
– 10g/s < air flow < 1kg/s
– 0.5g/s < fuel flow < 30g/s

The swirler components are shown in figure 2, with the swirler assembly in figure 3. The geometrical swirl number (S) was calculated based on the geometrical configurations as the ratio of the inlet angular to outlet axial momentum [7].

\[ S = \frac{\text{Axial flux of angular momentum}}{\text{Axial flux of axial momentum} \times \text{Exit Radius}} \]

The swirl number was calculated as 1.47.

A three dimensional model is used for the simulation. The complete system can be easily meshed by a tetrahedral unstructured mesh but it leads to higher number of elements generated which translates to longer computational times. However the solution is not stable for some viscous models. A hexahedral mesh was used to give fast and stable solutions. The simulation of the intake pipe starts just prior the swirl passage after a flame arrest protruded edge as shown in figure 4.a. The installation of the swirler in the combustion chamber and the grid is shown in figures 4.b and 5.

Figure 2 : The swirller components
Figure 3 : The swirller assembly

Figure 4 : Cross section showing the swirler installation
(a) The parts of assembled swirler used in simulation
(b) The installation of the swirler in the combustion chamber and the mesh of the whole system
Numerical Model

Laminar Flame Speed Calculations

Laminar flame velocity of a premixed flame is defined as the propagation velocity of a plane, undisturbed flame without heat loss and buoyancy effect. Although such flame may be difficult to produce experimentally, the definition is very suitable for numerical calculations using detailed kinetic reaction schemes. Laminar burning velocity is a constant; under specific pressure and temperature, that provides reliable data on global flame propagation.

Fuels such as methane and hydrogen very often serve as fuels for combustion studies in gas turbine. Therefore, there is a need for reliable data of burning velocities for these fuels at high pressure and preheat temperatures and at various equivalence ratios.

Peters et al. [35] considered methane, ethylene, ethane, acetylene, and propane flames, numerically generated burning velocities were approximated using an algebraic expression that had been derived for methane-air flames by asymptotic methods [36]. The approximation uses the inner layer temperature as an auxiliary variable and thereby provides a means of calculating effective Zel'dovich numbers as a function of equivalence ratio, pressure, and preheat temperature. Their work is extended to include n-heptane, iso-octane, and methanol in [37, 38]. They also report predictions of the response of laminar premixed flames to stretch, characterized by Markstein numbers, for methane, ethylene, ethane, propane, and iso-octane/air flames. The Markstein number predictions are compared with measurements reported by others. A technique is described by Kwon et al. [39] to eliminate this difficulty of comparison between the results in [37, 38] and those of other authors.

By this method of approximation, the burning velocities of lean methane-air mixtures can be calculated in the range of preheat temperatures between 298 K and 800 K and pressures between 1 bar and 40 bar. The equation that can be used for the burning velocity $S_L$ of stoichiometric methane-air flames has the general form

$$S_L = A(T^0) Y_{F,u}^m T_u \left( \frac{T_b - T^0}{T_b - T_u} \right)^n$$

(1)

where, $T^0$ is the inner layer temperature, representing the crossover temperature between chain-branching and chain-breaking reactions. Within the temperature profile of a premixed flame it marks the transition from the inert preheat zone to the reaction zone, and it is therefore the point where the second derivative vanishes and the slope is maximum. The function $A(T^0)$ only depends on thermodynamic and kinetic properties and $Y_{F,u}$ is the mass fraction of the fuel in the unburnt gas. The temperatures $T_u$, and $T_b$ are those in the unburnt and the burnt gas, respectively. m and n are constants for the fuel.
The relation between the inner layer temperature and the pressure and the function \( A(T^0) \) are approximated as

\[
p = B \exp\left( -\frac{E}{T^0} \right)
\]

or simply

\[
T^0 = \frac{E}{\ln \frac{B}{p}}
\]

and,

\[
A(T^0) = F \exp\left( -\frac{G}{T^0} \right)
\]

And the adiabatic flame temperature can be calculated for lean flames as:

\[
T_b = aT_u + b + c\phi + d\phi^2 + e\phi^3, \quad \phi \leq 1
\]

The parameters for methane and hydrogen:

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**Hydrogen/Methane Laminar Flame Speed**

If \(\text{H}_2/\text{CH}_4\) blend is considered as a fuel with hydrogen and methane mole fractions \(n_{\text{H}_2}\) and \(n_{\text{CH}_4}\) respectively then the hydrogen volumetric fraction \(\gamma\) is defined as:

\[
\gamma = \frac{n_{\text{H}_2}}{n_{\text{H}_2} + n_{\text{CH}_4}}
\]

Sarli and Benedetto [1] calculated the laminar burning velocities of hydrogen–methane/air mixtures at NTP conditions using the CHEMKIN PREMIX code with the GRI kinetic mechanism. Their results show that the values of the blends laminar burning velocities are always smaller than those obtained by averaging the laminar burning velocities of the pure fuels according to their molar proportions. The linear combination of the laminar burning velocity of the pure fuels can be calculated as follows:

\[
S_{\text{L,linear}}(\phi, \gamma) = \gamma \cdot S_{\text{L,H}_2}(\phi) + (1 - \gamma) \cdot S_{\text{L,CH}_4}(\phi)
\]

where \(S_{\text{L,H}_2}\) and \(S_{\text{L,CH}_4}\) are the laminar burning velocity of hydrogen and methane evaluated at the same equivalence ratio of the hybrid fuel (\(\phi\)).

It appears that the computed values of the mixture laminar burning velocity are always well below those obtained by averaging the flame speeds of the constituent gases in molar proportions. This implies the presence of strong non-linear effects in chemical kinetics that emphasize the weight of the more slowly reacting methane in the composite fuel combustion. Moreover, in lean mixtures the hydrogen addition enhances the methane reactivity slightly, while a strong inhibiting effect of the hydrogen substitution by methane is observed at rich conditions.

A correlation for evaluating the laminar burning velocity of hydrogen–methane/air mixtures at NTP conditions as a function of equivalence ratio and fuel composition has been proposed by Yu et al. [34] for hydrogen mole fraction in the fuel up to 0.7. The authors have been able to linearly correlate the laminar burning velocity of the hybrid flames with the burning
velocity without hydrogen addition and a single parameter indicating the extent of the hydrogen content. More precisely, hydrogen has been considered to be present only in stoichiometrically small quantities, its combustion requiring four times less oxygen than methane. Consequently, they have assumed that there is enough air to facilitate a complete oxidation of hydrogen, while the remaining air is used to oxidize methane. An effective methane/air equivalence ratio, \( \phi_F \), has been therefore defined as follows:

\[
\phi_F = \frac{C_F / (C_H / C_A)}{(C_F / C_A)_{st}},
\]

while the relative amount of hydrogen addition, \( R_H \), has been expressed according to

\[
R_H = \frac{C_H + C_H / (C_H / C_A)_{st}}{C_F + [C_F - C_H / (C_H / C_A)_{st}]}.
\]

where \( C_A \), \( C_F \) and \( C_H \) are the initial mole fractions of the air, methane and hydrogen, respectively (the subscript ‘st’ denotes the stoichiometric conditions). In the explored ranges of \( \phi_F \) (0.51-1.37) and \( R_H \) (0-0.5), the laminar burning velocity \( (S_L) \) has been then correlated by the following equation:

\[
S_L(\phi_F, R_H) = S_L(\phi_F, 0) + 0.8R_H \text{ (m/s)}
\]

More recently, El-Sherif [40] has numerically reproduced the experimental results by Yu et al. [34] at \( \phi_F \) ranging from 0.62 to 1.2 and \( R_H \) varying up to 0.4. In this parameter range he has proposed the following correlation:

\[
S_L(\phi_F, R_H) = 0.38\phi_F^{0.35} \exp[-5.5(\phi_F - 1.1)] + 0.84R_H \text{ (m/s)}
\]

with \( \phi_F \) and \( R_H \) defined according to (8) and (9), respectively.

Eq. (11) is similar to Eq. (10), but it presents the explicit dependence of the laminar burning velocity without hydrogen on the fuel/air equivalence ratio \( (\phi_F) \). Eqs. (10) and (11) are able to take into account the linear trend of the laminar burning velocity with hydrogen addition on the methane rich side. Due to the expressions of the parameters \( \phi_F \) and \( R_H \) defining the composition of the hybrid fuel/air mixtures, these equations are intrinsically valid only for low hydrogen contents.

Another correlation for laminar burning velocities of \( \text{H}_2/\text{CH}_4 \) mixture was proposed by Liu et al. [41]. The correlation uses Le Chatelier’s Rule-like formula that can be expressed according

\[
S_{L,LC}(\phi, \gamma) = \frac{1 - \gamma}{S_{L,H2}(\phi) + \gamma S_{L,CH4}(\phi)}
\]

where \( S_{L,H2} \) and \( S_{L,CH4} \) are the laminar burning velocity of hydrogen and methane evaluated at the same equivalence ratio of the hybrid fuel \( (\phi) \).

Sarli and Benedetto [1] tested the feasibility of a Le Chatelier’s Rule-like formula at different values of inlet pressure (1, 5 and 10 atm) and temperature (300, 350 and 400 K), respectively. A good prediction is obtained, except for rich mixtures with high hydrogen contents. With this limitation, the proposed formula is successfully applied also to mixtures at higher than normal values of initial pressure (up to 10 atm) and temperature (up to 400 K). They do think that the Le Chatelier’s Rule-like formula (1) is able to take into account the kinetic interaction between radicals. However, at rich conditions when dealing with high hydrogen (and then H radicals) contents the interaction is too strong to be reproduced by Eq. (1) and a more sophisticated formula is required.
**Calculation of Laminar Flame Speed in Fluent**

Both premix and partially premix models require the laminar flame speed as a material property even if the combustion model is considered as adiabatic or non-adiabatic. Laminar flame speed depends strongly on the composition, temperature, and pressure of the unburnt mixture. For perfectly premixed systems, the reactant stream has one composition, and the laminar flame speed is approximately constant throughout the domain. However, in partially premixed systems, the laminar flame speed will change as the reactant composition (equivalence ratio) changes, and this must be taken into account.

Accurate laminar flame speeds are difficult to determine analytically, and are usually measured from experiments or computed from 1D simulations. FLUENT uses fitted curves obtained from numerical simulations of the laminar flame speed [37, 38]. These curves were determined for hydrogen ($\text{H}_2$), methane ($\text{CH}_4$), acetylene ($\text{C}_2\text{H}_2$), ethylene ($\text{C}_2\text{H}_4$), ethane ($\text{C}_2\text{H}_6$), and propane ($\text{C}_3\text{H}_8$) fuels. They are valid for inlet compositions ranging from the lean limit through unity equivalence ratio (stoichiometric), for unburnt temperatures from 298 K to 800 K, and for pressures from 1 bar to 40 bars.

FLUENT fits these curves to a piecewise-linear polynomial. These flame speed fits are accurate for air mixtures with pure fuels of $\text{H}_2$, $\text{CH}_4$, $\text{C}_2\text{H}_2$, $\text{C}_2\text{H}_4$, $\text{C}_2\text{H}_6$, and $\text{C}_3\text{H}_8$. If an oxidizer other than air or a different fuel is used, if the mixture is rich, or if the unburnt temperature or pressure is outside the range of validity, then the curve fits will be incorrect. So, it is not possible to run with the values of laminar flame speed that are calculated by default for other fuels that are not mentioned before, mixtures leaner than the lean limit or richer than the rich limits, and/or mixtures that have conditions outside the specified pressure and temperature limits.

The laminar flame speed must be specified by using another source such as experimental measurements or chemical kinetics software with detailed 1D simulations. The required inputs are values for the mean mixture fraction at 10 laminar flame speeds. The minimum and maximum mixture fraction limits for the laminar flame speed are the first and last values of $f$ that are input.

**CHEMKIN-PRO software package for calculation of the laminar burning velocity**

An unstretched laminar burning velocity of methane and methane/hydrogen flames has been calculated using CHEMKIN-PRO [42] software package. CHEMKIN-PRO consists of a set of different application models, which are used to solve various chemical kinetic problems. “Flame Speed Calculator” reactor model has been used to determine the laminar speed of one-dimensional freely propagating flame. PREMIX [43] code, which has been developed by Sandia National Laboratories, has been used to run this model.

“Flame Speed Calculator” model with “Parameter Study Facility” option has been utilised to perform the numerical burning velocity calculations. The model simulates a freely propagating flame in which the point of reference is a fixed position on the flame, thus the flame speed is defined as the velocity of unburned gas moving towards the flame [42]. This model uses mixture averaged transport properties with correction velocity formulation. Equivalence ratio has been chosen as variable parameter. A number of runs have been performed for different temperature and pressure conditions. The domain length of 10 cm has been specified and the grid of 200 points has been selected, which has facilitated faster convergence. Adaptive grid control parameter based on gradient $\text{GRAD} = 0.1$ and adaptive grid control parameter based curvature $\text{CURV} = 0.1$ have been selected. Initial grid based on temperature profile estimate has been specified. Mixture averaged transport, correction velocity formalism with automatic estimation of temperature profile options have been used.
Different kinetic models should be used for different gas mixtures as no one mechanism can be considered as universal model for all possible gas mixtures. GRI-Mech [44] mechanism is often used in the research of methane and methane based gases combustion. It considers 53 species and 325 elementary reactions. This mechanism has been developed to investigate methane and natural gas flames and has been validated extensively at various pressure and temperature conditions. The researchers have reported that this mechanism could also be suitable to some extent for biomass gasification-derived producer gas [45], methane hydrogen mixtures [46, 47] and for hydrogen air mixtures [48, 49] at atmospheric conditions. However there have been larger discrepancies observed between experimental data and numerical calculations using GRI-Mech kinetic mechanism for pure and diluted hydrogen at higher pressures [48, 50].

There are several kinetic mechanisms, developed for the combustion application of hydrogen. O’Conaire et al. mechanism has been developed to simulate the combustion of hydrogen and oxygen in a variety of combustion environments and over a wide range of temperatures, pressures and equivalence ratios. O’Conaire kinetic mechanism comprises of 8 species and 19 elementary reactions. The temperature ranges from 298 to 2,700 K, the pressure from 0.05 to 87 atmospheres, and the equivalence ratios from 0.2 to 6. Ströhle and Myhrvold reported [48] that Li et al. [51] and O’Conaire et al. [50] chemical kinetics mechanisms provide much accurate results in comparison with experimental data at elevated pressures, and GRI-Mech underpredicts laminar flame speed considerably. They also showed that the San Diego [52] mechanism yields reasonable results for helium diluted high pressure hydrogen flames. Lafay et al. [53] have utilised the GRI-Mech and San Diego mechanisms to calculate flame thickness. They have proved that these mechanisms are in good agreement with the experimental data at the atmospheric conditions at equivalence ratios above 0.55. Sarli and Benedetto [1] found that the GRI-Mech kinetic mechanism, used in their simulation, underpredicted laminar burning velocity at high hydrogen content in the methane-hydrogen mixture. They identified three different regimes in flame propagation depending on hydrogen mole fraction in fuel mixture.

Taking into account the research reports it has been decided to use different mechanism for different methane/hydrogen fuel mixtures. GRI-Mech mechanism has been used for methane/hydrogen with hydrogen content up to 50%, because it is believed that methane combustion kinetics prevail in the combustion process. San Diego mechanism has been chosen for the investigation of methane – hydrogen mixtures with the hydrogen content above 50%, because it has been showed [48] that this mechanism predicts hydrogen laminar flame speed more accurately at elevated pressures. O’Conaire at el. mechanism has been utilised for laminar flame speed calculation for pure hydrogen, as its accuracy has been supported by various researchers [48, 50].

Premixed Combustion Modelling and Flashback analysis

Computational Fluid Dynamics (CFD) is widely used in the last decade in many engineering applications. CFD can be used to predict internal and external flows which have several applications in heat transfer, fluid mechanics, combustion, and chemistry. The rapid development in hardware/software technology helps to generate commercial CFD codes that become a vital component in the design of industrial products and processes. There are many reasons to model a combustion system. The most obvious is to gain insight into various configurations in order to improve performance [54, 55].

Premixed Combustion Modelling

In premixed combustion, fuel and oxidizer are mixed at the molecular level prior to ignition [56]. Combustion occurs as a flame front propagating into the unburnt reactants. Premixed combustion is much more difficult to model than non-premixed combustion. The reason for this is that premixed combustion usually occurs as a thin, propagating flame that is stretched...
and contorted by turbulence. For subsonic flows, the overall rate of propagation of the flame is determined by both the laminar flame speed and the turbulent eddies. The laminar flame speed is determined by the rate that species and heat diffuse upstream into the reactants and burn.

The flame front propagation is modelled by solving a transport equation for the density-weighted mean reaction progress variable, denoted by \( c \) [57]:

\[
\frac{\partial}{\partial t} (\rho c) + \nabla \cdot (\rho \mathbf{u} c) = \nabla \cdot \left( \frac{\mu_t}{Sc_t} \nabla c \right) + \rho S_c \tag{13}
\]

Where
- \( c \) = mean reaction progress variable
- \( Sc_t \) = turbulent Schmidt number
- \( S_c \) = reaction progress source term (s\(^{-1}\))

The progress variable is defined as a normalized sum of the product species,

\[
c = \frac{\sum_{i=1}^{n} Y_i}{\sum_{i=1}^{n} Y_{i,eq}} \tag{14}
\]

Where
- \( n \) = number of products
- \( Y_i \) = mass fraction of product species \( i \)
- \( Y_{i,eq} \) = equilibrium mass fraction of product species \( i \)

Based on this definition, \( c = 0 \) where the mixture is unburnt and \( c = 1 \) where the mixture is burnt.

The value of \( c \) is defined as a boundary condition at all flow inlets. It is usually specified as either 0 (unburnt) or 1 (burnt).

The mean reaction rate in equation (1) is modelled as

\[
\rho S_c = \rho_u U_t |\nabla c| \tag{15}
\]

Where
- \( \rho_u \) = density of burnt mixture
- \( U_t \) = turbulent flame speed.

The turbulent flame speed is computed using a model of wrinkled and thickened flame fronts:

\[
U_t = A (u')^{3/4} U_1^{1/2} \alpha^{-1/4} \ell_t^{1/4} = A \left( \frac{\tau_t}{\tau_c} \right)^{1/4} \tag{16}
\]

Where
- \( A \) = model constant
- \( u' \) = root-mean-square (RMS) velocity (m/s)
- \( U_1 \) = laminar flame speed (m/s)
- \( \alpha = \kappa / \rho c_p \) = molecular heat transfer coefficient of unburnt mixture (thermal diffusivity) (m\(^2\)/s)
- \( \ell_t \) = turbulence length scale (m)
- \( \tau_t = \ell_t / u' \) = turbulence time scale (s)
- \( \tau_c = \alpha / U_1^2 \) = chemical time scale (s)

The turbulence length scale \( \ell_t \) is computed from

\[
\ell_t = C_D \left( \frac{u'}{\varepsilon} \right)^3 \tag{17}
\]
Where $\varepsilon$ is the turbulence dissipation rate.

The model is based on the assumption of equilibrium small-scale turbulence inside the laminar flame, resulting in a turbulent flame speed expression that is purely in terms of the large-scale turbulent parameters. The default values of 0.52 for $A$, 0.37 for $C_D$ are recommended by Zimont et al. [57], and are suitable for most premixed flames.

Non-adiabatic premixed combustion model is considered. The energy transport equation is solved in order to account for any heat losses or gains within the system. These losses/gains may include heat sources due to chemical reaction or radiation heat losses.

The energy equation in terms of sensible enthalpy, $h$, for the fully premixed fuel is as follows:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot \left( k \left( \frac{k + \varepsilon}{c_p} \nabla h \right) + S_{h,\text{chem}} + S_{h,\text{rad}} \right)$$

(18)

$S_{h,\text{rad}}$ represents the heat losses due to radiation and $S_{h,\text{chem}}$ represents the heat gains due to chemical reaction:

$$S_{h,\text{chem}} = \rho \bar{S}_c H_{\text{comb}} Y_{\text{fuel}}$$

(19)

where

$S_c$ = normalized average rate of product formation (s$^{-1}$)

$H_{\text{comb}}$ = heat of combustion for burning 1 kg of fuel (J/kg)

$Y_{\text{fuel}}$ = fuel mass fraction of unburnt mixture

**Turbulence Modelling**

The turbulence model that is used is the shear-stress transport (SST) $k$-$\omega$ model, so named because the definition of the turbulent viscosity is modified to account for the transport of the principal turbulent shear stress. It has feature that gives the SST $k$-$\omega$ model an advantage in terms of performance over both the standard $k$-$\omega$ model and the standard $k$-$\varepsilon$ model. Other modifications include the addition of a cross-diffusion term in the $\omega$ equation and a blending function to ensure that the model equations behave appropriately in both the near-wall and far-field zones [56].

The SST $k$-$\omega$ model has a similar form to the standard $k$-$\omega$ model. The turbulence kinetic energy, $k$, and the specific dissipation rate, $\omega$, are obtained from the following transport equations:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k \mathbf{u}_i) = \frac{\partial}{\partial x_j}(\Gamma_k \frac{\partial k}{\partial x_j}) + G_k - Y_k + S_k$$

(20)

and

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \omega \mathbf{u}_i) = \frac{\partial}{\partial x_j}(\Gamma_\omega \frac{\partial \omega}{\partial x_j}) + G_\omega - Y_\omega + D_\omega + S_\omega$$

(21)

Where

$G_k$ represents the generation of turbulence kinetic energy due to mean velocity gradients. $G_\omega$ represents the generation of $\omega$. $\Gamma_k$ and $\Gamma_\omega$ represent the effective diffusivity of $k$ and $\omega$, respectively. $Y_k$ and $Y_\omega$ represent the dissipation of $k$ and $\omega$ due to turbulence. $D_\omega$ represents the cross-diffusion term. $S_k$ and $S_\omega$ are user-defined source terms. Calculations for all previous terms have been fully described in [56].
Results and Discussion

Laminar Flame Speed

The laminar burning velocities of hydrogen–methane/air mixtures at different pressures and temperatures were calculated by varying the equivalence ratio from lean to rich conditions and the fuel composition from pure methane ($\gamma=0$) to pure hydrogen ($\gamma=1$).

The calculation results of methane hydrogen mixtures at elevated temperatures and pressures using GRI-Mech and San Diego kinetic mechanisms are presented in figure 6. The results of GRI-Mech and San Diego mechanisms are almost identical for the 70% methane and 30% hydrogen mixture. At higher hydrogen amount in the mixture GRI-Mech underpredicts flame speed. This supports similar findings of other researchers [48]. The discrepancies between these two models can be observed in the region of equivalence ratio below 1 and above 1.4, although in the region from 1 to 1.4 GRI-Mech produces slightly higher flame speed results in comparison with San Diego mechanism.

![Figure 6](image)

Figure 6. CHEMKIN-PRO calculated laminar flame speed of methane hydrogen mixtures at 7 bara and 673 K. Numbers represent hydrogen amount in the mixture; SD – San Diego mechanism, GRI – GRI-Mech mechanism.

Similar comparison has been done for pure hydrogen. The results of the calculations are presented in figure 7. Three mechanisms: O’Conaire et al. mechanism, San Diego mechanism and GRI-Mech, have been compared at 7 bara 473 K and 673 K. O’Conaire et al. mechanism has been developed to simulate the combustion of hydrogen and oxygen in a variety of combustion environments and over a wide range of temperatures, pressures and equivalence ratios.

GRI-Mech mechanism underpredicts hydrogen flame speed in the region of equivalence ratio up to 1 and above 1.5 in comparison with O’Conaire mechanism. San Diego mechanism predictions are more accurate in comparison with GRI-Mech. O’Conaire mechanism predicts the highest flame speed.
Figure 7. CHEMKIN calculated laminar flame speed of hydrogen at 7 bara 473 K and 673 K; O’Con – O’Conaire mechanism, SD – San Diego mechanism, GRI – GRI-Mech mechanism.

For pure methane and pure hydrogen, the laminar flame speed was calculated by CHEMKIN at 1.01325, 3 and 7 bar each at 300, 473 and 673 K. GRI-Mech mechanism was used for CH$_4$ laminar flame speed calculations while O’Conaire et al. mechanism is used for H$_2$. The results are shown in figure 8.a for methane and figure 8.b. for hydrogen. It is recognized that the laminar flame speed increases as the temperature increases but decreases with pressure. This is applicable for both CH$_4$ and H$_2$ up to the stoichiometric mixture ratio ($\phi$=1) but for H$_2$ rich mixture, the pressure proportionality is not applicable.

A comparison between the laminar flame speed values arising from Chemkin and Fluent analysis is performed at the same pressure and temperature range stated above for both CH$_4$ and H$_2$. The results are shown in figure 9. It was found that the values appear to be within about ± 10 % deviation for lean mixtures up to the stoichiometric mixture ratios. For rich mixtures Fluent produces higher predicted values compared to Chemkin. Chemkin results are taken to be more accurate so it is used for establishing a PDF table for turbulent combustion and flashback analysis in the next section.
Figure 9. Comparison between laminar flame speed values calculated by CHEMKIN and FLUENT at various pressures and temperatures for (a) CH₄, (b) H₂
Chemkin is used to calculate the laminar flame speed for hybrid fuels containing H₂/CH₄ blends. A new approximation is suggested for calculating the laminar flame speed of H₂/CH₄ blends. This approximation is based on using linear correlation of the laminar burning velocities of the pure compositions with respect to the mixture gravimetric analysis. The blend laminar flame speed then can be calculated as follows:

\[ S_{L_{linear}}(\phi, g) = g_{H2} \cdot S_{L_{H2}}(\phi) + (1 - g_{H2}) \cdot S_{L_{CH4}}(\phi) \]  

(22)

where \( S_{L_{H2}} \) and \( S_{L_{CH4}} \) are the laminar burning velocity of hydrogen and methane evaluated at the same equivalence ratio of the hybrid fuel (\( \phi \)), whilst \( g_{H2} \) is the mass fraction of hydrogen in H₂/CH₄ mixture.

\[ g_{H2} = \frac{m_{H2}}{m_{H2} + m_{CH4}} \]  

(23)

where \( m_{H2} \) and \( m_{CH4} \) are the mass fractions of hydrogen and methane respectively.

The values of H₂ mass fraction at which calculations are performed are tabulated in table 1.

Table 1: Mole fraction and corresponding mass fraction of hydrogen in H₂/CH₄ blends

<table>
<thead>
<tr>
<th>H₂ Mole fraction (( \gamma ))</th>
<th>H₂ Mass Fraction (( g_{H2} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.15</td>
<td>0.021583</td>
</tr>
<tr>
<td>0.30</td>
<td>0.050847</td>
</tr>
<tr>
<td>0.50</td>
<td>0.11111</td>
</tr>
<tr>
<td>0.70</td>
<td>0.225806</td>
</tr>
<tr>
<td>0.85</td>
<td>0.414634</td>
</tr>
<tr>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

A comparison is performed between CHEMKIN (C), the asymptotic method (A) described by equations 1 to 5 incorporated with Le Chatelier’s Rule-like correlation stated by equation 12, and the new approximation (N). The results are shown in figure 10 for different pressures, temperatures and equivalence ratios for the full range of H₂/CH₄ blends from pure methane up to pure hydrogen. A good prediction for laminar flame speed by using the new approximation is demonstrated especially at 1 atm and for methane-dominated combustion region i.e. up to \( \gamma \) equals 0.5. The results of the new approximation are still acceptable at high pressure as the deviation is limited to about 15% of the Chemkin values.
Figure 10. Comparison between three methods for calculating the laminar flame speed for H₂/CH₄ hybrid fuel at different pressures, Equivalence ratios, and temperature.

Flashback Results

Flashback Determination

The segregated fluent solver was always used for the simulation of premixed combustion. The swirl burner gives good flame stabilization, but can produce Central Recirculation Zones (CRZs) that extend back over the central fuel injector, allowing the flame to propagate into this region. This can be largely eliminated by fitting a sharp step to the exhaust nozzle of the burner and helps to reduce flashback. The boundary conditions are chosen to be 700 K for all walls. Simulations were not sensitive to this value apart from the exit tip of the burner. The default under relaxation factor was chosen.

In order to provide more insight, two parameters are suggested for normalizing the results. The first parameter is the relative mass flow rate \( m_r \) which is defined as:

\[
m_r = \frac{m}{m_{FB}}
\]  

(24)
where \( m \) is the mass flow rate of the combusting mixture and \( m_{ofB} \) is the mass flow rate at which flashback occurs for stoichiometric methane/air mixture at the standard ambient conditions (1 atm and 25°C).

The second parameter is the relative velocity (\( U_r \)) which is defined as

\[
U_r = \frac{U}{U_{ofB}}
\]

(25)

where \( U \) is the average axial velocity at the burner exit which is calculated from the total mass flow rate and the density of the mixture at isothermal conditions. \( U_{ofB} \) is the average axial velocity at the burner exit at which flashback occurs for stoichiometric methane/air mixture at the standard ambient conditions (1 atm and 25°C).

Flashback is defined as the combusting of the premixed mixture of air and fuel before entering the combustion chamber i.e., in the swirler or supply line. To determine flashback, reference values for mass flow rate and velocity to be used for results normalization, a number of complete runs are performed using methane/air with stoichiometric mixture ratio at standard atmospheric conditions. The mass flow rate is changed until flashback occurs. The difference between the mass flow rate in the case of normal combustion without flashback and that with flashback is less than 0.1% of the former. The temperature and progress variable contours of the two cases are shown in figure 6. The first figure 11.(a) shows normal combustion. Combustion develops within the combustion chamber and there is no combustion in the swirler section as the temperature is still low and the progress variable (c) equals zero. Figure 11.(b) shows flashback. Combustion extended upstream and the temperature is raised inside the swirler passage due to combustion. The progress variable moved up to 1 inside the swirler.

![Figure 11. Flashback determination for stoichiometric CH₄ mixture at the standard ambient conditions (1 atm and 298K).](image)

(a) Normal Combustion at relative mass flow of 1.005  
(b) Flashback at relative mass flow of 0.997

To define the flashback limits at each equivalence ratio, many runs were performed. As shown in figure 12, two different regions of operation are recognizable. The first region above the curve is the region where combustion is stable without flashback. The second region is the region below the curve in which flames are unstable with flashback. Flashback peaks at an equivalence ratio of unity, whilst operation under lean mixture conditions is clearly favorable.
Figure 12. Flash determination for methane/air combustion at atmospheric pressure and mixture temperature of 300 K at various equivalence ratios.

CH$_4$ Combustion and Flashback

To study the effect of pressure, complete sets of runs were performed at pressures of 1.01325, 3 and 7 bar respectively, the initial mixture temperature was 673 K, and results are shown in figures 13A and B. In figure 13A the correlation between the relative mass flow rate and the equivalence ratio is shown at different pressures. The operating total mass flow rate required to avoid flashback increases with pressure. However, figure 13B shows that the relative velocity at which the flashback exists is a weak function of pressure, typically reduced by about 15% moving from 1.0 bar to 7.0 bar.

In the same way, the effect of temperature on the stability limits was studied. Complete sets of runs were performed at three different temperatures of 300, 473 and 673 K for an operating pressure of 1.01325 bar. Figure 14A and 14B show the correlation between the relative mass flow rate and velocity with equivalence ratio at different temperatures. Flashback increases as the air preheat temperature increases in both figures 14A and 14B. The velocity at which the flashback occurs is a strong function of temperature, typically increasing by about 8 moving from 300 K to 673 K.
Figure 13. The effect of pressure variation on the stability limits for CH$_4$ combustion at various equivalence ratios and, A) The corresponding relative mass flow rates; B) the corresponding relative velocity at which flashback occurs.

Figure 14. The effect of temperature variation on the stability limits for CH$_4$ combustion at various equivalence ratios and, A) The corresponding relative mass flow rates; B) the corresponding relative velocity at which flashback occurs.

$H_2$/CH$_4$ mixtures and Flashback

Combustion of a premixed fuel mixture containing ($\gamma$ H$_2$ + (1-$\gamma$) CH$_4$) was simulated from $\gamma$ = 0 up to 1 with flashback occurring under some conditions. The simulation is performed under atmospheric pressure and 300 K. As what was done to determine the flashback limits for methane, a complete set of runs was also performed to determine flashback limits at each H$_2$ mole fraction in the hybrid fuel. The results are shown in figure 15 for different equivalence ratios. It is found that the flashback tendency for H$_2$/CH$_4$ is always taking the same trend for the laminar flame speed as it is shown in figures 10 and 15. The flashback tendency, represented by the relative mass flow rate and relative velocity shown in figure 15, increases with the increase of H$_2$ content in the mixture. The increase in flashback tendency doesn't follow a linear correlation from pure methane up to pure hydrogen. There are three regimes
which can be identified in the hybrid blend flashback map depending on the hydrogen mole and mass fractions in the fuel. These three regimes are:
(1) methane-dominated combustion (0 < \( \gamma < 0.5 \)) \( \equiv (0 < g_{H_2} \leq 0.1) \) mass fraction;
(2) transition (0.5 < \( \gamma \leq 0.89 \)) mole fraction \( \equiv (0.1 \leq g_{H_2} \leq 0.5) \) mass fraction; and
(3) methane dominated by hydrogen combustion (0.89 < \( \gamma < 1 \)) mole fraction \( \equiv (0.5 \leq g_{H_2} < 1) \) mass fraction.
In both regimes (1) and (3) the flashback tendency increases linearly with increasing the hydrogen molar content of the blend. In regime (1), the enhancement of the methane flashback tendency by hydrogen addition is slight. In regime (3) methane substitution to hydrogen has a significant decreasing effect on flashback. So, if the flame stability is considered when talking about H\(_2\) additions to CH\(_4\) it is better to work in the first region of methane-dominated combustion. It is confirmed that the lean mixtures have more resistance to flashback than stoichiometric mixtures.

Figure 15. Flashback tendency map for H\(_2\)/CH\(_4\) combustion represented by relative mass flow rate and relative velocity for full range of hybrid fuel.
Conclusions

This paper has presented novel results showing the application of a number of methods for calculating laminar flame speeds for a range of fuels ranging from pure methane to pure hydrogen, with a wide range of blends in between. It is shown that considerable non-linearities exist between various blends owing to changes in the chemical mechanisms as the fuel blends changes. Methods are developed to overcome these problems. The results have then been applied to the design of a generic swirl burner to be used in gas turbine applications where flashback needs to be considered in the context of low NOx, lean premixed units.

For the device in question it is shown that flashback can be characterised by an average exhaust velocity which is a function of the fuel type, inlet air temperature and more weakly the pressure. Maps are developed which indicate stable and unstable operating conditions

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