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BURNER DEVELOPMENT AND OPERABILITY ISSUES ASSOCIATED WITH STEADY FLOWING SYNGAS FIRED COMBUSTORS

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This article addresses the impact of syngas fuel composition on combustor blowout, flashback, dynamic stability, and autoignition in premixed, steady flowing combustion systems. These are critical issues to be considered and balanced against emissions considerations in the development and operation of premixed combustors. Starting with blowout, the percentage of hydrogen in the fuel is suggested to be the most significant fuel parameter, which is more fundamentally related to the hydrogen flame's resistance to stretch induced extinction. Turning to flashback next, it is shown that multiple flashback mechanisms are present in swirling flows, and the key thermophysical properties of a syngas mixture that influence its flashback proclivity depend upon which flashback mechanism is considered. Flashback due to turbulent flame propagation in the core flow and the interaction of heat release with pulsations are less critical, whereas flame propagation in boundary layers and flashback due to the interaction of the heat release with vortex breakdown dynamics are most significant. Then, combustion instability is considered. The key flame parameter impacting the conditions under which instabilities occur is the spatial distribution of the flame. As such, fuel composition influences dynamics through impacts upon flame speed and the flame stabilization point. Furthermore, certain syngas fuel compositions are not more inherently stable than others – rather, each mixture has particular islands in the parameter space of, e.g., velocity and fuel/air ratio, at which instabilities occur. Changes in fuel composition move these islands around but do not necessarily eliminate or introduce instabilities. Relative to autoignition, measurements indicate that the ignition delay time exceeds typical premixer

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residence times, though by a substantially less margin than suggested by the calculations. Recent experiment work suggest that current detailed kinetic mechanisms developed for hydrogen/carbon monoxide ignition overestimate the ignition delay time, indicating the need for additional kinetic work in the low temperature, high pressure regime.

Keywords: Autoignition; Blowoff; Combustion; Flashback; Instability

INTRODUCTION

This article reviews the scientific issues associated with operating steady flowing combustors on syngas, such as gas turbines, boilers, and furnaces. A number of important practical problems must be dealt with in developing a combustion system capable of combusting syngas, particularly if the system must also emit low levels of CO and NO_x emissions (Richards et al., 2001). Some of these issues are well understood and utilize well-developed engineering knowledge, such as required line or orifice sizes needed to pass a given fuel flow rate in order to supply the combustor with a given heating rate (Klimstra, 1986). There are a number of other issues, however, substantially less well understood, which involve complex interactions between fundamental combustion phenomenon and fluid mechanics. In particular, burners involve complex, poorly understood interactions between swirling flow dynamics, flow field alterations induced by volumetric expansion across the flame, and flame propagation. In related fashion, there are a number of operability issues related to operating the combustor in a safe, efficient, and reliable manner. This includes having the combustor reliably hold the flame so that it neither flashes back nor blows out, and burns the fuel in a “quiet,” steady fashion. We briefly review four of the most critical of these operability issues below, all of which are strongly influenced by fuel properties:

Blowout refers to situations where the flame becomes detached from the location where it is anchored and is physically “blown out” of the combustor. Blowout is often referred to as the “static stability” limit of the combustor. Blowoff involves the interactions between the reaction and propagation rates of highly strained flames in a high speed, often high shear flow. Blowoff events can require a lengthy and often expensive system shut down, purge cycle, and restart.

A second issue is *flashback*, where the flame propagates upstream of the region where it is supposed to anchor and into premixing passages that are not designed for high temperatures. Flashback involves turbulent flame speed propagation in a highly inhomogeneous, swirling flow. Since premix nozzles are not well cooled, flame flashback is a serious safety risk. After flashback has occurred, flame anchoring in the nozzle leads to a fast rise of material temperatures, with subsequent overheating and failure.

Combustion instability refers to damaging pressure oscillations associated with oscillations in the combustion heat release rate. These oscillations cause wear and damage to combustor components and, in extreme cases, can cause liberation of pieces into the hot gas path, damaging downstream turbine components.

Autoignition refers to the homogeneous ignition of the reactive mixture upstream of the combustion chamber. Similar to flashback, it results in chemical reactions and hot gases in premixing sections, but its physical origins are quite

different from those of flashback. Rather than the flame propagating upstream into the premixing section, autoignition involves spontaneous ignition of the mixture in the premixing section.

Understanding these operability issues requires understanding of more fundamental combustion properties. While significant levels of fundamental understanding on the flame propagation and the stability characteristics of lean, premixed systems has been gained in conventionally fueled, natural gas-air systems, little is known about these issues for alternate gaseous fuels. Furthermore, the majority of the fundamental investigations of the combustion characteristics of these synthetic gases are for nonpremixed flame configurations (Barlow et al., 2000; Correa and Gulati, 1988a; Drake, 1986; Correa and Gulati, 1988b; Masri and Dibble, 1988).

As discussed in the first article of this volume, syngas fuels are typically composed primarily of H_2 , CO, and N_2 , and may also contain smaller amounts of CH_4 , O_2 , CO_2 , and other higher-order hydrocarbons. Depending upon the source and particular processing technique, these fuels can have significant ranges in relative composition of these constituents. A compilation in Moliere (2002) shows that the volumetric H_2/CO ratio varies from a low of 0.33 to a high of 40, the percentage of diluent gases (e.g., N_2 , CO_2 , Ar) from 4–51%, and the percentage of water from 0–40%.

The current generation of premix burners designed for operation with natural gas cannot be reliably operated with syngas. For this reason, syngas in gas turbines is presently combusted in non-premixed flames using special burner designs, which differ substantially from natural gas burners (Huth et al., 1998). If low NO_x emissions are required, the peak combustion temperature is controlled using large amounts of water and/or nitrogen for dilution of the fuel. Burning syngas in a non-premixed mode with less than 25 ppm NO_x (@15% O_2) in heavy-duty gas turbines requires dilution of the fuel to at least 7500 MJ/kg (Döbbeling et al., 1996) or even lower heating values (Huth et al., 1998). Although premixing offers many advantages over dilution, attempts to improve fuel flexibility of natural gas premix burners for gas turbines has had only limited success so far, because of the operability issues highlighted in this article. The objective of this article is to compile known results and discuss their implications on each of these operability issues. This is intended to provide an overview of current understanding of the underlying processes that must be considered when evaluating how a given combustor's operability will be affected with syngas fuel.

DISCUSSION

Blowout

Developing physics-based correlations of blowout behavior is complicated by lack of understanding of the detailed phenomenology of the blowout process, such as the dynamics of near blowoff flames or the flame characteristics at the stabilization point (Durbin and Ballal, 1996). For example, there is disagreement on whether premixed flames in high turbulent intensity gas turbine environments have flamelet, "thickened" flamelet, or well stirred reactor (WSR)-like properties. This has implications on blowout modeling, because the appropriate physical model clearly

changes depending whether the reaction zone exhibits flame sheet or volumetric characteristics.

Methods for developing blowout correlations in the latter case (i.e., using WSR scaling ideas) have been studied extensively. Several different theories or physical considerations have been used in past blowout correlation studies, such as those of Zukoski and Marble (1997), Spalding (1955), or Longwell et al. (1953). As noted by Glassman (1996), these lead to similar correlations that relate the blowoff limits to a Damköhler number, i.e., ratio of a residence and chemical kinetic time, τ_{res}/τ_{chem} .

$$Da = \frac{\tau_{res}}{\tau_{chem}} \quad (1)$$

As such, for a given flow field, parameterized by τ_{res} , the key combustion parameter influencing blowoff limits is a chemical kinetic time scale. Figure 1 plots the dependence of a calculated chemical time, defined as $\tau_{chem} = \alpha/S_L^2$, upon the $H_2/CO/CH_4$ ratio, where α and S_L denote the thermal diffusivity and laminar flame speed, respectively. Each point in the composition space corresponds to a fixed adiabatic flame temperature of 1500 K; i.e., the mixture stoichiometry is adjusted for each composition such that the mixture has the given temperature. Note the order of magnitude variation in chemical time from the fast H_2 mixtures to the slower CO mixtures.

The preceding observation is very consistent with experimental findings that the key parameter that influences the blowout/extinction characteristics of syngas is the percentage of hydrogen. Numerous studies have shown that the fuel/air ratio at which blowoff/extinction occurs monotonically decreases as the percentage hydrogen in the fuel increases, whether it is CH_4/H_2 mixtures (Schefer, 2003), CO/H_2 mixtures (Vagelopoulos and Egolfopoulos, 1994), or other hydrogen-blended fuels. For example, the data presented in Figure 2 is reproduced from Zhang et al. (2007), and plots the dependence of the fuel/air ratio at blowoff of $H_2/CH_4/CO$ mixtures upon the percentage of H_2 in the fuel. These plots show the well known result that, in general, mixtures can be stabilized with lower equivalence ratios as the H_2 concentration

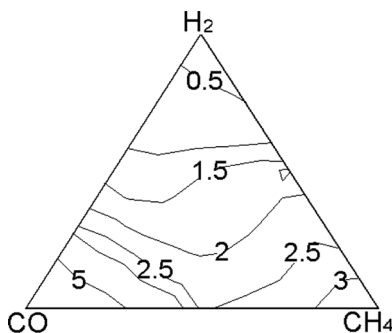


Figure 1 Dependence of chemical time (ms), calculated using GRI3.0 as the kinetic mechanism, upon fuel composition at fixed adiabatic flame temperature, 1500 K at 1.7 atm with 300 K reactant temperature.

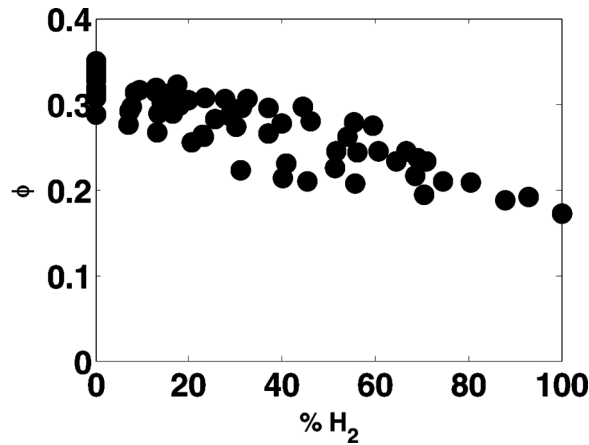


Figure 2 Measured dependence of equivalence ratio of $\text{CH}_4/\text{H}_2/\text{CO}$ mixtures at LBO upon H_2 mole fraction at nozzle exit velocity of 59 m/s, reactants temperature 458 K and combustor pressure 4.4 atm (Zhang et al., 2007)

increases. Although this graph focuses on fuel/air ratio at blowoff, this data can be replotted to illustrate similar trends for adiabatic flame temperature or laminar flame speed, whose blowoff values also monotonically decrease with fuel/air ratio.

While clearly there are important issues such as appropriate choice of length and velocity scale, Damköhler number scalings have been found to capture blowout trends across a wide range of fuel compositions up to about 50% H_2 , as illustrated by Figure 3. These data consist of a number of permutations of $\text{CO}/\text{H}_2/\text{CH}_4$ fuel blends, ranging from pure fuels to various combinations. The Damköhler number

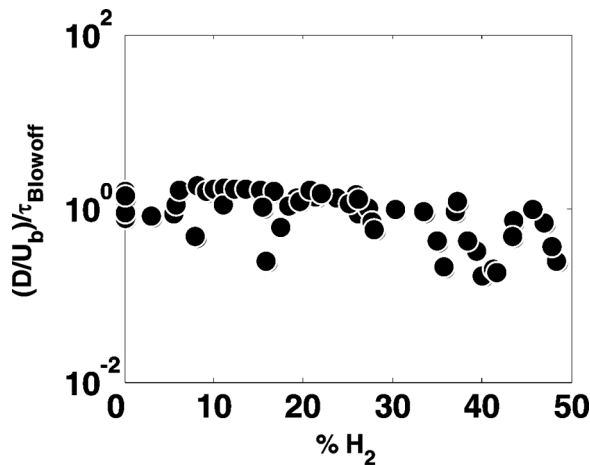


Figure 3 Ratios between residence time and chemical time at constant nozzle exit velocity of 59 m/s, combustor pressure of 1.7 atm, and 300 K reactant temperature.

is defined as

$$Da = \frac{\tau_{res}}{\tau_{Blowoff}} = \frac{D/U_b}{\tau_{Blowoff}} \quad (2)$$

where D , U_b denote the width of the combustor and the burned flow speed, respectively. The chemical time scale $\tau_{blowoff}$ equals the calculated residence time at blowoff of a well-stirred reactor model (using the GRI 3.0 mechanism), which correlates well with the time scale used in Figure 1 (Zhang et al., 2005).

While scatter is present in the data, the results show that blowout occurs at a roughly constant value of the Damköhler number. However, as noted by Noble et al. (2006), the Damköhler number at blowoff changes by four orders of magnitude in fuels with 50–100% H_2 . Noble et al. (2006) suggested that this variation might be a manifestation of thermal diffusive/flame stretch effects, with the result that the fuel/air ratio, and therefore the chemical time, with which to characterize the mixture, ϕ_{mod} , was not the globally averaged fuel/air ratio, ϕ_{ave} , but a modified fuel/air ratio, $\phi_{mod} = \phi_{ave} + f(D_f/D_{ox})$, where D_f and D_{ox} denote the fuel and oxidizer diffusivity.

However, such efforts to correlate blowoff limits with a single, constant time scale probably passes over key physics. For example, the residence time parameter, assumed constant above, would certainly be expected to change somewhat as the underlying fluid mechanics of these flames changes due to the variation in burned gas temperature, and therefore burned gas flow velocity and Reynolds number. Furthermore, observations by Zhang et al. (2005) suggest that the physical mechanisms of blowoff change with hydrogen levels. For mixtures with H_2 levels below about 50% by volume, the blowoff event occurs abruptly with a small change in fuel composition, although sometimes preceded by slight liftoff of the flame from the burner. However, for high H_2 mixtures, the blowoff and liftoff events were quite distinct. Usually, the flame became visibly weaker, lifted off from the holder, and moved progressively downstream with decreases in equivalence ratio before blowing off for good.

In addition, a variety of recent studies by Muruganandam et al. (2005) and Nair and Lieuwen (2005), have shown that flames do not generally blow off in a completely discontinuous manner. Rather, as blowoff is approached, the flame becomes increasingly unsteady, lifts off the burner, and moves downstream. These observations were quantified by acoustic and/or optical measurements of the chemiluminescence/sound radiated by the flame, which show increasingly large fluctuations, characterized by time localized “events” in the signal as blowoff boundary is approached.

These fluctuations in chemiluminescence apparently are associated with axial fluctuations in the leading edge of the flame and localized extinction in the flame, in which holes in the flame sheet occur in response to high localized stretch. The unburned fuel passes through the hole and either passes out of the combustor, or is burned downstream. This alters the local fluid mechanics that, in turn, influences the stretch rate that the flame is subjected to at a later instant of time. Measurements of Zhang et al. (2007) have shed some light on the underlying mechanisms for this

unsteadiness in a CH_4/H_2 fueled, swirl combustor. In their facility, the flame was nominally attached to an annular centerbody under stable conditions, see Figure 4.

Much of the near blowoff dynamics was associated with the flame periodically detaching from the centerbody and blowing downstream. This process repeated itself in a chaotic fashion—PIV images showing the flow field and flame at four instances of time are shown next. In a non-reacting swirling flow such as this one, it is known that the flow field is characterized by complicated, three dimensional helical structures and precessing vortices (Syred, 2006). Note that when the flame is firmly attached, the downstream flow field exhibits essentially none of these features. When the flame is detached from the centerbody, these flow instabilities develop, as clearly shown in the figure. In this case, the flame is buffeted by a much more complex, vortical flow field.

Presumably, this detachment of the flame from the centerbody is due to the high shear at this location which, below some equivalence ratio, is larger than the extinction strain rate that the flame can withstand. Higher hydrogen flames, being able to withstand a higher strain rate than CH_4 at the same flame temperature (Sankaranand and Im, 2003; Ren et al., 2001), could remain attached to the centerbody for a broader range of fuel/air ratios – this partially explains why they

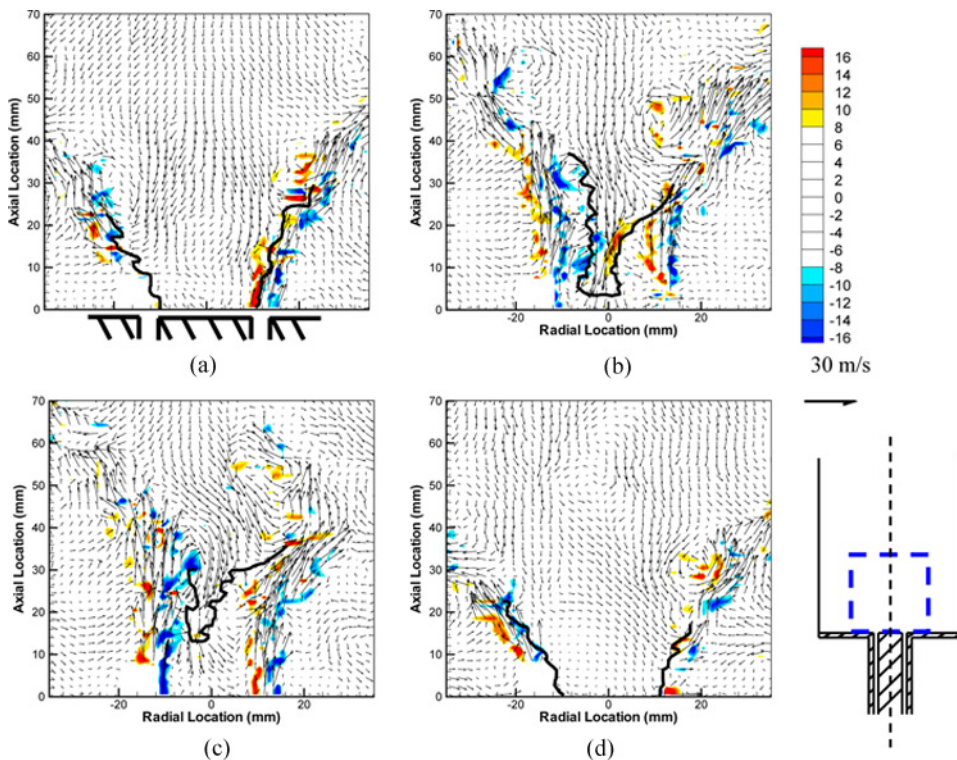


Figure 4 Snapshots of instantaneous flow field and flame front for 50% CH_4 / 50% H_2 flame near blowoff; bottom right schematic shows interrogation window (Zhang et al., 2007).

can persist at lower fuel/air ratios. However, due to vortex breakdown, an alternative flame stabilization point also exists downstream. For reasons that were not understood, the low H_2 flames did not persist in this downstream region, whereas the much higher H_2 flames could.

As such, while it is well established that percentage of hydrogen in the fuel plays a key role in its blowoff resistance, more work is needed to improve understanding of the dynamics of near blowoff flames and the blowoff phenomenology itself. As noted above, this is a highly dynamic, three-dimensional process, involving coupled interactions between the fluid mechanics and an extinguishing/reigniting flame. While experimental visualizations of these phenomena are helpful, given the complex topology of the flame and flow, a full understanding of this phenomenon will require detailed computational simulations and the resultant three-dimensional visualizations of the flame and flow that they enable.

Flashback

Flashback occurs when the turbulent flame speed exceeds the flow velocity along some streamline, allowing the flame to propagate upstream into the premixing section. While flashback is a classical topic that has been extensively investigated, its complexity increases substantially in swirling flows. In particular, experimental investigations have revealed *four* entirely different flashback mechanisms, which may lead to fast upstream flame propagation depending on the specific burner design and operating point: *turbulent flame propagation in the core flow*, *flashback due to combustion instabilities*, *flashback in the boundary layer*, and *flashback in the core flow due to alteration of vortex breakdown dynamics* (Kiesewetter, 2003; Kröner and Sattelmayer, 2003, 2004; Thibaut and Candel, 1998). The first three types can occur in swirling as well as non-swirling premix burners, whereas the fourth mechanism requires a swirling flow in the mixing zone. Importantly, fuel composition effects influence these mechanisms very differently. Each mechanism is considered separately below.

Turbulent Flame Propagation in the Core Flow. In a well-designed burner, flame propagation into the burner is prevented by high axial flow velocities. In principle, the flame will be able to propagate upstream in all zones of the burner with flow velocities below the turbulent burning velocity of the mixture. Flashback occurs when the turbulent flame speed exceeds the flow velocity along some streamline, allowing the flame to propagate into the premixing section (Plee and Mellor, 1978). This fact leads to the very simple design rule that the flow field must not have strong local velocity deficits and that the axial flow velocity must be *substantially* above the turbulent flame speed, S_T . Given the typical combustor pressure drop of $\Delta p_{tot} = 2\text{--}3\%$, absolute velocities are on the order of $u_{abs} \approx 90\text{--}120$ m/s in the burner mixing zone.

In the case of strong swirl, the axial velocity component drops to approximately $u_{ax} \approx 65\text{--}85$ m/s for the same burner pressure drop. The average turbulence level depends mainly on the swirl number in the mixing zone, although there is also some influence of the specific burner design; e.g., high swirl designs usually used in natural gas fueled systems have turbulence levels up to $u'/u_{abs} \approx 10\text{--}15\%$. Hence, typical

velocity fluctuations in premix burners are $u'/u_{ax} \approx 14\text{--}22\%$ or $u' \approx 9\text{--}18\text{ m/s}$. Assuming that the flow field is well designed and does not have local wakes with low axial velocity and with excessive turbulence, this leads to the conclusion that flame propagation in the turbulent burner core flow can only occur if the turbulent burning velocity is substantially higher than the characteristic turbulent velocity fluctuation. For the worst case of maximum swirl, the criterion for flame propagation is then $S_T/u' \approx 4.5\text{--}7$, and the reduction of the swirl number leads to even higher values.

Laminar flame speeds of high hydrogen syngas fuels are substantially higher than those of natural gas, and decrease with pressure. For engines without recuperation, pressure ratios above 15 and adiabatic flame temperatures $T_{ad} < 1900\text{ K}$, the laminar flame speed of syngas does not exceed $S_L = 2\text{ m/s}$, whereas recuperated engines with low pressure ratio of approximately 4 may reach $S_L = 4\text{ m/s}$.

It has been shown that the turbulent flame speed, S_T , exhibits a dependency upon fuel composition (Lipatnikov and Chomiak, 2005). For this reason, calculations of S_T by extrapolating data from other fuels that have similar laminar flame speeds S_L and from experiments with similar turbulence intensities u'/S_L , is not applicable. For example, Kido et al. (2002) measured the turbulent flame speed for a variety of H_2 , CH_4 , and C_3H_8 mixtures with nominally the same laminar flame speeds, but found variations in S_T that approached a factor of 10.

The reasons for these fuel effects are uncertain. Some workers have suggested that they can be correlated with thermo-diffusive effects. For example, differences in the relative rates of mass diffusion of the deficient species and/or thermal-diffusion affect the local laminar flame speed and the tendency of the flame to become spontaneously wrinkled, even in the absence of turbulent fluctuations. If differential diffusion processes are significant, then this could be expected to be significant in syngas fuels, because of the large differences in diffusivity of the various fuel and oxidizer components. If the turbulence level is very low this effect may become significant in syngas flames as the hydrogen concentration increases, but it may be less important in highly turbulent flames. We refer the reader to the comprehensive review on this subject by Lipatnikov and Chomiak (2005) for more discussion of this topic. Worst case estimates can probably be provided without considering preferential diffusion, as highly turbulent flow fields provide the worst-case scenarios for flashback due to turbulent flame propagation in the core flow.

If the simple relationship $S_T \approx S_L + u'$ is used, which does not account for the above effects, estimates for the turbulent flame speed S_T can be derived. This leads to $S_T/u' < 1.3$ in the non-recuperated case and to $S_T/u' < 1.5$ for the worst-case with intense recuperation. Since these values are substantially lower than $S_T/u' \approx 4.5\text{--}7$ required for flame propagation against the main flow velocity even in highly swirling case (see above), there is no indication that the drop of the flow speed below the turbulent burning velocity is the most critical cause of flashback. However, high turbulence levels, which are beneficial because they improve the fuel-air mixing and lead to shorter flames, clearly deteriorate the safety margin against flashback. For fuels with low laminar flame speeds S_L the margin is sufficiently large, because the turbulent flame speed S_T does not substantially exceed the characteristic turbulent velocity fluctuation u' , whereas this margin is smaller for the combustion of syngas. This drop may become critical if the velocity field has strong wake, high

turbulence regions from, e.g., swirler vanes, upstream separation zones and fuel jets. Consequently, a reduction of the swirl below the level usually employed in natural gas burners appears beneficial for the combustion of fuels with high hydrogen content, because this measure reduces turbulence and the turbulent flame speed, S_T .

In summary, a major design criterion for nozzle aerodynamics is that the axial velocity must be as high and as uniform as possible and free of strong wakes. As this criterion is important in the entire mixing zone and not only near the burner exit, designs with constant or with slightly conical and accelerating air flow paths downstream of the swirler are the preferred solution. Strong acceleration of the flow bears the danger of flame stabilization upstream near the fuel injector in stoichiometric zones near the fuel jets, in the event that the flame can propagate through the high velocity area downstream, such as during compressor surge.

Combustion Pulsation-Induced Flashback. A second flashback mechanism occurs through velocity fluctuations in the burner associated with combustion instabilities. At high pulsation levels the velocity field in the burner is substantially modulated. This modulation leads to the periodic drop of the flow velocity below the time average, and the generation of large scale vortices. If the frequency is low enough, the flame will propagate upstream. Although this basic mechanism is independent of fuel type *per se*, the pulsation level at which it becomes significant is a function of the “steady state” flashback margin described above. As such, this critical pulsation amplitude decreases with increases in hydrogen concentration of the syngas. However, since high pulsation levels must be avoided for other reasons mentioned in the section on combustion instabilities, flashback due to the second mechanism should not occur in regular, stable combustor operation. Its significance stems from the fact that unexpected combustion instabilities do lead to catastrophic burner failure due to flashback triggered by the pulsations.

Flashback in the Boundary Layer. Flashback in *laminar* boundary layers is a classical topic that has been extensively investigated (Lewis and von Elbe, 1987; Putnam and Jensen, 1948; Wohl, 1952). An investigation of boundary layer flashback in laminar, syngas fueled Bunsen flames has been detailed by Davu et al. (2005). Near the wall, the low velocities, as well as the boundary layer turbulence, promote flame propagation upstream. These effects compete with flame quenching due to the heat loss of the burner wall and flame stretch. As flashback limits in laminar flows correlate with the velocity gradient at the wall, the concept of the *critical velocity gradient* has been developed in the past. In laminar flow, this gradient g_f correlates with the laminar burning velocity S_L and a quenching distance d_p :

$$g_f \propto S_L/d_p \quad (3)$$

The quenching distance d_p is the characteristic length scale for the region at the wall, where the chemical reaction quenches due to heat losses. Scaling this quenching distance by a quantity on the order of the flame thickness, α/S_L leads to the following criterion for assessing the influence of the fuel on flashback in the boundary layer

$$g_f \propto S_L^2/\alpha \quad (4)$$

This expression shows that an increase of the laminar flame speed has a substantial influence on the critical velocity gradient required for flashback prevention. Moreover, the influence of pressure can be estimated; note that $\alpha \sim 1/p$. A quantitative evaluation of Equation (4) shows that the required velocity gradient for syngas with high hydrogen content is approximately one order of magnitude higher than that for natural gas. This indicates that boundary layer flashback concerns are much more critical for syngas than natural gas.

Whether the critical wall gradient in turbulent boundary layers is higher than in the laminar case, depends on the thickness of the quenching distance with respect to the laminar sublayer (Schäfer, 2005; Wohl, 1952). If the quenching distance is smaller, then the situation is similar to the laminar case. In the opposite, not yet extensively investigated case, an increase may be observed because thermal diffusion normal to the burner wall is increased by turbulence. Although flame propagation in turbulent boundary layers has not yet been fully explored, there are indications that proper aerodynamic burner designs produce substantially larger velocity gradients than required to avoid flashback for low flame speed fuels. However, the same conclusion cannot be made for fuels with high hydrogen content. In conclusion, burners with flow fields suited for the reliable premixing of natural gas may be prone to flashback in the boundary layer with high H_2 fuels. Another difficulty is that the addition of small amounts of air along the wall using an effusion technique, which has proven to be an effective measure against flashback for natural gas, may not dilute the mixtures outside the lean flammability limit in the critical near wall zones for hydrogen containing syngas. Even with dilution, the flame speed near the wall may be substantially higher than for natural gas without dilution.

Keeping the boundary layers as thin as possible is an essential design criterion for syngas burners and, even more important, local separation zones in the mixing zone must be avoided. Particularly critical are diffuser sections near the burner exit, which lead to a rapid increase of the wall boundary layers.

Vortex Breakdown Driven Flame Propagation in the Core of Swirling Flows. As opposed to boundary layer flashback, which is largely driven by flame propagation processes, a fourth mechanism is largely driven by the interaction of the heat release with swirling flows, which leads to a transition of the vortex breakdown characteristics (Kröner and Sattelmayer, 2003, 2004). Since in gas turbine combustion, swirling flows are almost exclusively used for flame stabilization, this fourth mechanism is of major relevance for premixed syngas burners.

A related mechanism has been discussed within the framework of studies on flame acceleration in spinning tubes (Umemura and Tomita, 2001). Essentially the same phenomenon, referred to as “combustion induced vortex breakdown” (CIVB), was observed in a tubular premix burner without centerbody (Figure 5) and it was found to be responsible for flame flashback in swirling flows with high axial velocities (Kröner and Sattelmayer, 2004).

A similar effect is observed in burners with a centerbody. In burners of this type the recirculation zone jumps suddenly back over the tip of the centerbody and propagates upstream forming an annular bubble.

For a given geometry, the dependence of the breakdown conditions depends upon swirl number. No breakdown occurs for low swirl numbers, $S < \sim 0.5$, and

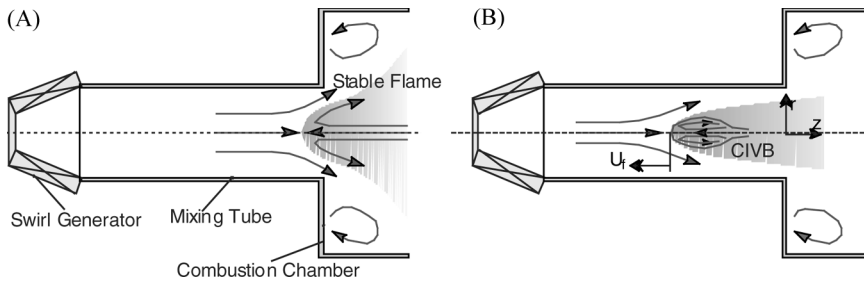


Figure 5 Flashback due to combustion induced vortex breakdown (CIVB): stable flame (A), flame moving upstream with the breakdown bubble (B).

only vortex breakdown states are present for high swirl numbers, $S > \sim 1$. However, these two regimes are separated by an intermediate hysteresis regime where either flow state is possible. As such, for intermediate swirl values which are typical of those used in practical systems (e.g., $S \sim 0.6$ – 1.2) the system has two possible states: no vortex breakdown or vortex breakdown (Brown and Lopez, 1990; Wang and Rusak, 1997). Nominally, no breakdown occurs in the nozzle, but combustion can provide the finite amplitude perturbation required to move the system from one flow state (no breakdown) to the breakdown state. The basic phenomenon leading to the sudden flow transition is that the flame contributes to vortex breakdown, and therefore generates a region of low or negative flow velocity ahead of it. The flame advances forward, causing the location of the vortex breakdown region to advance farther upstream into the mixing zone. This process continues as the flame proceeds farther and farther upstream. In this case, flashback can occur even if S_T is everywhere much less than the flow velocity in the isothermal case.

This basic effect depends upon the distribution of gas dilatation along the flame front which, in turn, depends upon the heat release; i.e., it is largely independent of chemical kinetic details (Noble et al., 2006). This is because gas expansion across the flame perturbs the approach flow and post flame streamlines, with a magnitude that is proportional to the density ratio across the flame and the relative inclination angle of the flame and approach flow (Noble et al., 2006).

However, kinetic effects enter through quenching of the flame as it propagates upstream. Kröner et al. (2007) measured the flashback limits of mixtures of natural gas and hydrogen and found a strong dependence on hydrogen content. They concluded that CIVB induced flashback is a more severe problem for strain resistant fuels, such as high hydrogen syngas. Design rules for minimizing CIVB induced flashback are detailed in Burmburger et al. (2006).

Combustion Instability

Combustion instabilities are characterized by large amplitude pressure oscillations that are driven by unsteady heat release (Lieuwen and Yang, 2005). A necessary, but not sufficient, condition for an instability to occur is that the unsteady

pressure and heat release oscillations must be in phase (or, more precisely, that their phase difference is less than ninety degrees) – under these conditions, the heat release adds energy to the perturbation field (Rayleigh, 1945). Syngas composition variations primarily affect combustion instabilities by altering this phase angle.

In order to understand how variations in fuel composition affect the phase difference between pressure and heat release fluctuations, it is necessary to consider the specific mechanism responsible for the instability. Two mechanisms are known to be particularly significant in premixed systems: these are fuel/air ratio oscillations and vortex shedding (Ducruix, 2005; Zinn and Lieuwen, 2005). In the former mechanism, acoustic oscillations in the premixer section cause fluctuations in the fuel and/or air supply rates, thus producing a reactive mixture whose equivalence ratio varies periodically in time. The resulting mixture fluctuation is convected to the flame where it produces heat release oscillations after a certain convective time delay, τ_{conv} . The coupling of the premixer acoustics with the fuel system is also affected by the pressure drop across the fuel injector (that, in turn, can vary with the fuels volumetric heating value).

The vortex shedding mechanism, as its name suggests, is due to large scale, coherent vortical structures. These structures are the result of flow separation from flameholders and rapid expansions, shear layer rollup, and vortex breakdown in swirling flows. These vortices are convected by the flow to the flame, where they distort the flame front after a convective time delay, τ_{conv} , and thereby cause the rate of heat release to oscillate. A computed image showing this process is illustrated in Figure 6.

Fuel/air ratio oscillations and vortex shedding become important when the resulting heat release perturbation is in phase with the pressure fluctuation. Basically, the sequence of physical processes involved in this feedback loop is as follows: a pressure fluctuation in the combustor results in a velocity and pressure fluctuation in the nozzle that causes a perturbation in the fuel flow rate and/or the vorticity. This perturbation is convected to the flame where it produces a fluctuation in the rate of heat release and, in turn, a pressure fluctuation. While we refer

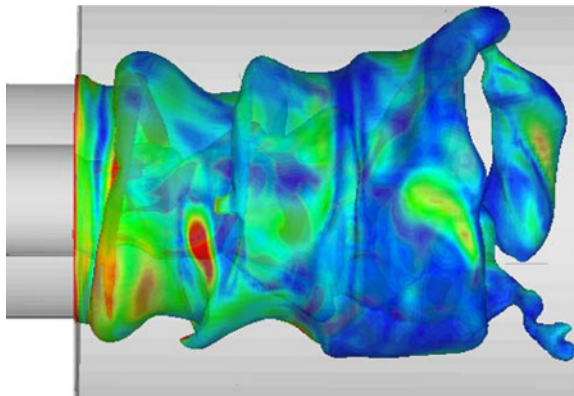


Figure 6 Computed image of swirling flame distorted by vortical structures, courtesy of Huang and Yang (2004).

the reader to other references for details (Lieuwen and Yang, 2005), this can be expressed by the following relationship:

$$\tau_{conv} + \tau_{chem} = kT \quad (5)$$

where τ_{conv} refers to the time required for either the equivalence ratio perturbation or the vortex to convect from its point of formation to the “center of mass” of the flame, τ_{chem} refers to the chemical delay time, T refers to the acoustic period, and k is an integer constant whose value depends upon the combustion chamber acoustics (Lieuwen et al., 2001; Gonzalez-Juez et al., 2005). The “center of mass” of the flame front, at least in terms of its phase response to perturbations is, in general a complex function of flame shape, flame length, flow velocity, and frequency. Only in the cases of low Strouhal numbers, defined roughly as the product of frequency and flame length, divided by the flow velocity, does this definition correspond to its general geometrical usage. While we raise this issue for the reader to be aware of it [see focused treatments on flame response transfer functions for a further discussion of this issue (Lieuwen, 2005)], we can nonetheless understand the leading order effects of syngas fuel composition by simply tracking their effect upon the flame location.

Variations in fuel composition impact the phase relationship expressed by Eq. (5) by affecting both the convective and chemical times. The effect of fuel composition on the chemical time is clear. The effect on the convective time can be better understood from the following equation, which expresses the convective time as the sum of the convective time in the premixer (τ_{pm}) and the convective time in the combustor (τ_{comb}):

$$\tau_{conv} = \tau_{pm} + \tau_{comb} \quad (6)$$

$$\tau_{conv} = [L_{pm}/u_{pm}] + [L_f/u_{comb}] \quad (7)$$

where L_{pm} refers to the distance from the point of origin of the disturbance to the entrance to the combustor, u_{pm} refers to the mean convective velocity in the premixer, L_f refers to the distance the perturbation travels from the combustor entrance to the “center of mass” of the flame, and u_{comb} refers to the mean convective velocity in the combustor.

The effect of variations in fuel composition on the convective time is primarily exercised through its influence upon the location of the flame “center of mass.” For example, increasing the percentage of hydrogen in a syngas fuel will increase the flame speed and therefore change the location of the flame “center of mass.” Of course, other parameters affecting the flame speed, such as inlet temperature and equivalence ratio, will also effect the flame location. To illustrate, we present in Figure 7 a set of data obtained by Figura et al. (2007) from an optically-accessible combustor which can be varied in length from 30 inches to 45 inches, corresponding to a range of acoustic frequencies from approximately 300 Hz to 400 Hz. The data are presented in the form of a two-dimensional stability map, which is a plot of the normalized rms pressure fluctuation versus the equivalence ratio and the combustor length. Results are shown for two fuels: (a) 100% natural gas and (b) 25%

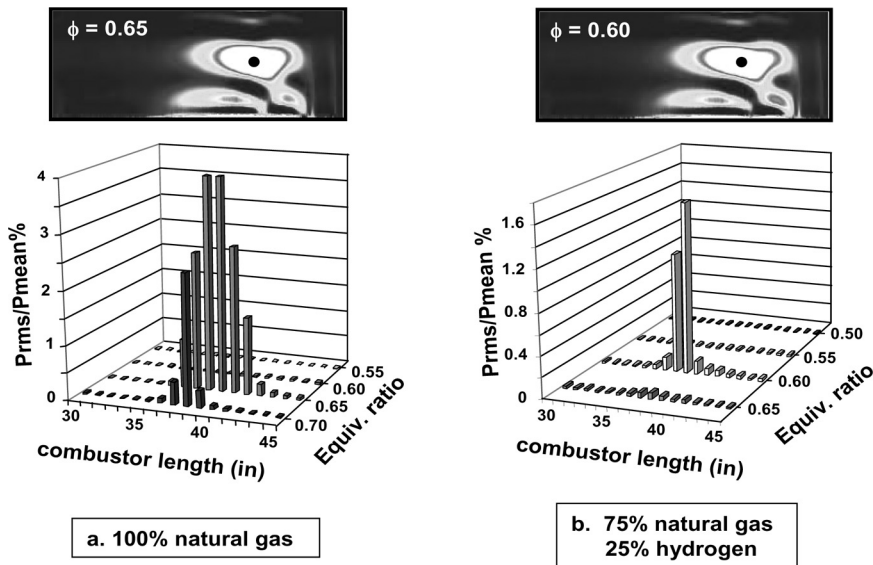


Figure 7 Instability maps and corresponding 2-D chemiluminescence flame structure images at an inlet temperature of 200°C and an inlet velocity of 75 m/s with (a) 100% natural gas fuel and (b) 25% hydrogen and 75% natural gas fuel (Figura et al., 2007).

hydrogen – 75% natural gas, and for a fixed inlet velocity and temperature of 75 m/s and 200°C.

The stability maps show that instabilities occur over a narrow range of combustor lengths and equivalence ratios for both fuels. In the case of 100% natural gas, the strongest instability occurs at an equivalence ratio of 0.65 and a combustor length between 38 and 39 inches, and has a frequency of 364 Hz. In the 25% hydrogen and 75% natural gas case, the strongest instability occurs at an equivalence ratio of 0.60 and a combustor length of 39 inches, and has a frequency of 352 Hz. Referring back to Eq. (7), and noting that the inlet velocity and the instability frequencies are nearly the same for both fuels, indicates that the distance to the flame “center of mass” must be nearly the same for both fuels at the operating condition where the instabilities occur. Confirmation of this is given in Figure 7, where the two-dimensional chemiluminescence flame images are shown for both fuels for the equivalence ratios where the instabilities occur. These images were taken under stable conditions, which were achieved by decreasing the length of the combustor to 30 inches. The flame images show that, as expected, the shape of the flame and the location of the flame “center of mass” (indicated by ●) is very nearly the same for both fuels. As discussed above, this can be explained by the fact that the increase in the flame speed, when hydrogen is added to the fuel, is offset by the fact that the instability occurs at a lower equivalence ratio.

Clearly, prediction of combustion instabilities is complex due to need for predicting relative values of driving and dissipation processes. Moreover, as shown in a number of recent studies, the flame response to perturbations, which determines the energy addition rate to the acoustic field by the flame, is quite complex. However, we

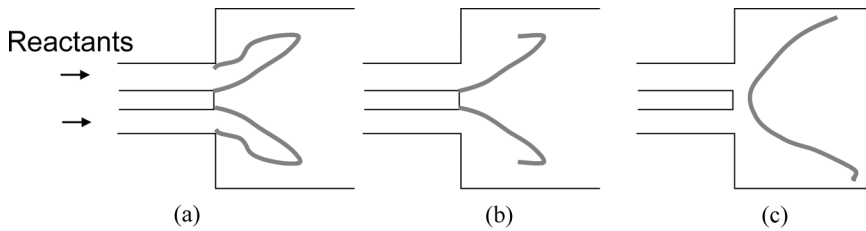


Figure 8 Schematic showing three possible flame configurations in a swirling flow, such as found in typical gas turbine combustors.

suggest that the key leading order effects of fuel composition can be understood from the above relatively simple characteristic time argument. In other words, understanding fuel composition effects upon combustion instability require an understanding of the flame length, flame attachment points, and possible downstream flame standoff location.

Even with these simplifications however, understanding these effects is quite complex. To illustrate, consider Figure 8, which plots three possible flame shapes typically observed in swirling flows – note that each flame configuration will have a different center of mass. In configuration (a), the flame is stabilized on the rapid expansion and centerbody. If the shear at these regions exceeds the extinction strain rate of the flame at one or both locations the flame will locally extinguish, detach and move downstream. Configuration (b), represents a situation where the flame can still stabilize at the centerbody, but the shear at the rapid expansion is too high. In configuration (c), the flame strain is too high at both points and the flame is stabilized by the vortex breakdown bubble farther downstream. Clearly, fuel composition will have significant impacts on which flame configuration is present, because of the strong dependence of extinction strain rate on hydrogen levels in the fuel. Furthermore, for a given flame configuration, the turbulent flame speed will have an important influence upon the flame length.

In addition, the fluid mechanics of the flow also exercise influences on the flame location. For example, the standoff location of the flame in configuration (c) will depend upon the vortex breakdown bubble location.

Finally, even relatively small variations in flame length, standoff location, or overall configuration can exert significant influences upon instabilities in low Mach number flows – this is due to the fact that the pressure-heat release phase is proportional to changes in the absolute value, as opposed to the relative value, in the ratio of the convective time to acoustic period, τ/T . To illustrate, note that a 45-degree pressure-heat release phase shift, $\tau/T = 0.12$, is induced by a variation in flame length or standoff distance of only 1.5 cm, assuming an axial velocity and frequency of 50 m/s and 400 Hz. This sensitivity grows with increases in frequency and decreases in velocity.

Autoignition

Typical inlet temperatures (600–900K) and pressures (5–35 atm) of gas turbines are sufficiently high for spontaneous ignition of many fuels. As such, designing the

premixer to avoid autoignition requires knowledge of the reactive mixture's ignition delay time and a residence time. In order to achieve uniform mixing, longer mixing times are desired – however, this obviously conflicts with the need to avoid autoignition. The time scale associated with physical mixing in current low emissions combustors is on the order of 1–5 msec, based on bulk velocities and premixer volumes. However, it should be recognized that the complex aerodynamics associated with swirl, separation, and strong gradients can make it difficult to assign a single time scale to represent the physical premixing time in a given system. Even if a very small fraction of the mixture has longer residence times, their spontaneous ignition can lead to ignition of the entire mixture within the premixer.

The key question then is whether the ignition delay time of the fuel being used at the local premixer conditions is longer, shorter, or about the same as the premixing time scale. If the ignition delay time is much longer than several milliseconds, concerns about autoignition may be allayed to some degree. Of course all aspects of the operation must be considered, such as startup or load shedding.

This question of whether the syn-gas/air mixture will autoignite in the premixer can be addressed both theoretically and experimentally. A number of kinetic mechanisms for hydrogen or hydrogen/carbon monoxide are available, yet there are only a handful of experimental results available for autoignition of hydrogen or hydrogen/carbon monoxide at compressor discharge conditions to confirm the accuracy of the models. For theoretical calculations, a number of mechanisms specific to hydrogen or hydrogen containing fuels have been published recently, which include Mueller et al. (1999a, b); Baulch et al. (1994); Akbar et al. (1997); Davis et al. (2005); San Diego Mechanism 2003/08/30 (Williams, 2003); and Hydrogen 2004 (O'Conaire et al., 2004). In addition, GRI-Mech 3.0 (Smith et al., 1999) is worth mentioning because it is ubiquitous in use for natural gas and commonly used in kinetic calculations. This final mechanism is optimized for methane and natural gas and so may not provide optimal results for hydrogen or hydrogen/carbon monoxide. The mechanisms are summarized in Table 1. Because establishment and improvement of mechanisms is an on-going efforts at many research facilities, evaluation of mechanisms for H_2/CO containing fuels is an important ongoing effort.

Given the tremendous amount of experience and anecdotal data on natural gas fired industrial gas turbines using lean premixed combustion strategies, it is helpful to assess the relative autoignition behavior of natural gas and hydrogen. For this assessment, simulations were carried out for H_2 and natural gas using appropriate mechanisms for each (Mueller et al., 1999a, b; Smith et al., 1999). Typical results are shown in Figure 9. The composition of NG used in the example is 80% CH_4 , 10% C_2H_6 , and 10% C_3H_8 on a volumetric basis. This result shows that ignition delay times for H_2 tend to be shorter than those of natural gas. Interestingly, the difference appears relatively small at temperatures below 1000 K (above 1000/T = 1.0). The differences are quite significant, however, as the temperature increases, especially above $T = 1250$ K (below 1000/T = 0.8). For ignition delay in premixing ducts in non-recuperated systems, the temperature ranges expected tend to be less than 1000 K, thus for gas turbine applications, the result shown in Figure 9 appears promising because it suggests that ignition delay times for hydrogen are comparable to those for natural gas. These delay times at gas turbine premixer conditions are 100 to 1000 msec. The non-linear behavior in the hydrogen case is due mainly to the

Table 1 Chemical reaction mechanisms for fuels containing H₂ and/or CO

Mechanism	Species	Reactions	Notes
Mueller et al. (1999)	13	34	Nitrogen containing elemental reactions not included, but are available
GRI-Mech 3.0 (Smith et al.)	53	325	Designed for natural gas with limited C3 content
Baulch et al. (1994)	42	167	Compiled by Kaneshige (1996)
San Diego 2003/08/03	39	173	Includes up to C3
Davis et al. (2005)	14	38	Updated versions under development
Hydrogen 2004, (O'Conaire et al., 2004)	10	21	No CO reactions

second explosion limit behavior (Yetter et al., 1992) of hydrogen oxidation. Such behavior is attributed to the depletion of the OH radical pool in favor of less-reactive HO₂ radicals (Skinner and Ringrose, 1965) The subtleties of mixture composition, temperature, and pressure, then, can become more complicated in the CH₄/H₂/CO system than it is for natural gas. In addition, it is known that the mechanisms commonly used for natural gas are not necessarily recommended for T < 1000 K. (Smith et al., 1999) As a result, though the ignition delay appears similar at low temperatures, this is based on calculations done at temperature that are really outside of the limits for which the mechanisms are felt to be reliable. Hence additional validation is in order.

Because pressure effects and actual delay times are important in gas turbine applications and because of non-linear behavior exhibited for some species like

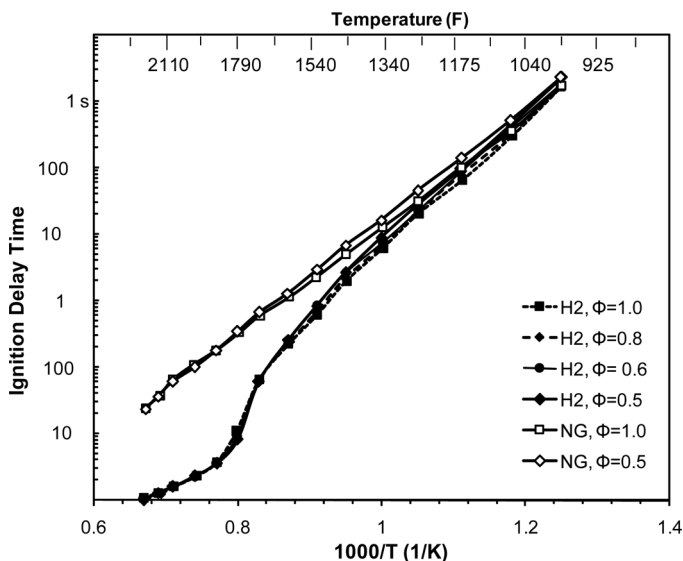


Figure 9 Calculated ignition delay time at 15 atm – pure hydrogen vs. natural gas (NG) at various equivalence ratios.

hydrogen as shown in Figure 9, there is considerable interest in further verifying the answers to the key question about the ignition delay time. While shock tubes are commonly used for such measurements (Spadaccini and Colket, 1994; Petersen et al., 1999; Huang et al., 2004), flow reactors have also been used, but on a much more limited basis (Mueller et al., 1999; Beerer et al., 2006; Beerer and McDonell, 2007). These two approaches tend to favor high temperature and low temperature, respectively.

Experimental studies for flowing syngas mixtures are very limited. Aside from work documented in a project report (Peschke and Spadaccini, 1985), no other results for syngas ignition delay at low temperatures are available. One limited study conducted resulted in a single ignition event (Boleda et al., 1998). Recently, results for hydrogen/carbon monoxide mixtures at low temperatures have been reported (Petersen et al., 2007). Herein, results obtained in a flow reactor are plotted against predictions using the Mueller mechanism for various pressures in Figure 10. Because the predicted ignition delay time determined using any number of recent mechanisms is similar (Beerler and McDonell, 2007; Petersen et al., 2007), results using a single representative mechanism are sufficient to make observations. Figure 10 shows the previous (Peschke and Spadaccini, 1985) and recent flow reactor data (Beerler et al., 2006) along with a plot of predicted delay times. The recent results coincide with the previous ones, which is most evident when pressure is corrected for. A pressure dependency of $P^{-0.75}$ is used, as reported previously (Peschke and Spadaccini, 1985). As shown, when the recent results are scaled using this relation, they lie directly on top of the previous results that were obtained for pressures between 12–23 atm. While the simulated delay times shows a shorter delay time for higher pressures in the lower temperature regions, in all cases the predictions are 1–2 orders

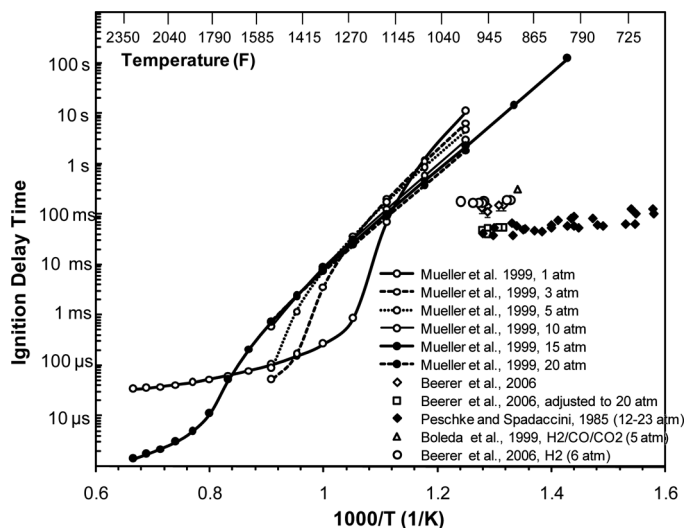


Figure 10 Comparison of existing and current ignition delay results for hydrogen/carbon monoxide mixtures: 50% H₂, 50% CO.

of magnitude longer than the measured values and diverge farther as temperature decreases.

Recent work using other ignition delay techniques also suggests that the differences observed between the models and the measurements at low temperature are real and not just a property of constant pressure flow reactors (Petersen et al., 2007; Walton et al., 2007). The significance of these discrepancies is more clearly illustrated in Table 2. Ignition delay times were calculated using the pressures, temperatures and fuel/air ratios of several gas turbine engines in commercial use today. Compressor discharge temperatures were obtained from the *International Turbomachinery Handbook 2006* or were estimated based on an isentropic compression to the desired pressure. Delay times were calculated using an experimentally obtained correlation (Peschke and Spadaccini, 1985), and secondly through homogeneous ignition calculations using the Mueller mechanism (Mueller et al., 1999).

Again, the discrepancies are significant. For example, for the GE 9H engine, the predicted ignition delay time is in the range of 11.8 seconds, while the experimental correlation predicts ignition in only 85 ms. Clearly, further studies are required to clarify this discrepancy and further underscore the need to better understand low temperature ignition behavior. The results also point out that caution is needed when applying different tools to assess this problem. The underlying assumptions contained within the comprehensive kinetic modeling (e.g., homogeneous ignition) may not apply in the case of flowing mixtures within gas turbine premixing ducts (or flow reactors). In reality, short ignition times have been observed for various experimental techniques, but often the objective of those experiment was to attain homogeneous ignition (which generally occurs at higher temperatures) and therefore the observed short times were not of direct interest (Beer and McDonnell, 2007b; Chaos and Dryer, 2007). Further complicating the analysis are impacts of contaminants, particulate, and possible surface chemistry all of which may contribute to the ignition process in practical applications.

Table 2 estimated ignition delay times for representative engine compressor discharge conditions

Engine	Premixer condition		Estimated ignition delay time of H ₂ /CO mixture (ms)	
	Pressure (atm)	Air Temp (K)	Flow reactor experiments (Peschke and Spadaccini, 1985; Beer et al., 2006)	Homogeneous ignition model (Mueller et al., 1999)
GE 9H*	23	705	85	11,800
Solar Taurus 65	15	670	153	— (**)
Solar Taurus 60	12.3	644	221	—
Solar Mercury 50**	9.9	880	59	4,941
GE LM6000*	35	798	35	34,850
Siemens V-94.3A*	17.7	665	141	—
Siemens V-94.2*	12	600	336	—
Capstone C-60**	4.2	833	140	—

*Inlet temperature estimated from ideal gas, isentropic compression.

**Recuperated engine.

***—indicates no ignition within 5 minutes.

CONCLUDING REMARKS

A number of challenges remain for future investigations to clarify these issues. Fundamental flame properties, such as laminar flame speeds, stretch sensitivities, and extinction stretch rates are largely unknown at the conditions of interest. Furthermore, more system dependent properties, such as turbulent flame speed, are also largely uncharacterized and critical factors such as the thermo-diffusive dependencies of these mixtures require clarification. In addition, the fluid mechanics of reacting swirl flows, which critically impacts all of these operability concerns is poorly understood and requires extensive further work. A large body of systematic work for non-reacting swirl flows exists at low Reynolds numbers, but a number of open questions remain about the swirl flow dynamics in high Reynolds number, reacting flow dynamics. Furthermore, these dynamics are strongly influenced by exothermicity impacts on the fluid mechanics.

As discussed, flame location appears to be more fundamentally influenced by the flame's ability to withstand the high strain, high shear regions. Relative to ignition delay, it is evident that more work is needed in the low temperature regime. Theoretical predictions suggest autoignition is not an issue with syngas, however, the experimental results suggest that this issue may be worth revisiting. Thus far, ignition delay times (at least in a 1D sense) suggest that this should not be a "show stopper." However, the safety margin observed approaches a factor of 10 in some cases and with uncertainties as to the potential role of surface chemistry and particulates or other contaminants, dismissing the potential for autoignition in lean premixed combustion of syngas is risky. As such, these problems will continue to be a rich area requiring further investigation in order to understand and predict these dynamic combustion phenomena.

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