Study of Syngas Combustion Parameters Effect on Internal Combustion Engine

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ABSTRACT
Syngas is considered to be a viable alternative fuel to fossil derived fuels in both gas turbines and reciprocating gas engines. Detail studies of syngas as a dual fuel in compression ignited engine, diesel as a pilot fuel and as a single fuel in a naturally aspirated spark ignited engines are found in the literature. Even though the prospect of fueling naturally aspirated spark ignition engine with syngas is very promising and even cost competitive with that of natural gas, it is associated with power de-rating that is mainly provoked by the decrease in volumetric efficiency. With the advancement in gasification technology and sten regulation with both fossil derived fuels and solid bio-energies, detail investigation of syngas’s combustion parameters and their effect in an internal combustion engine is very important. This study presents the combustion features like calorific value, laminar flame velocity and flammability limits of syngas in detail and their effects on the combustion in an internal combustion engine, spark ignition engine in particular. The study shows that understanding of the combustion characteristics of syngas is very important to investigate the effect of diluting inert gases on the overall performance and emission. The fact that the proportion of the constituent gases of syngas produced from gasification varied with variation of input parameters, there is limitation in the characterization of both laminar flame speed and flammability limit.

Key words: Syngas, calorific value, laminar velocity, flammability limit, combustion

INTRODUCTION
Energy consumption for transport is the main sector which is heavily dependent on liquid and gaseous fuels, out of this gasoline takes the major share. Gasoline is generally represented by C\textsubscript{n}H\textsubscript{8n}, where n is a number that allows the molecular weight to reach 105-110. The H-C ratio, 1.85 for gasoline, is very important factor in the greenhouse gas emission. An increase in the H to C ratio leads to less production of CO\textsubscript{2} and more production of H\textsubscript{2}O in the combustion products. It is because of this reason substitution of gasoline with high H-C ratio fuels like methane and syngas from natural gas feedstock, is preferred. On the other hand, solid fuels mainly biomass and coal are abundantly available. They were the key energy source in the industrial revolution era fueling iron ore furnaces, steam boilers and engines and locomotive engines, but they were replaced by liquid and gaseous fuels in the last 50 years because of their harmful pollutant emission and the penalty for their low flexibility.
Advancement in conversion technologies from solid to liquid or gaseous fuels and scarcity of the conventional fossil fuel are two drivers leading a reviving interest to use solid fuels as a source of energy globally. Among the conversion technologies, gasification is promising and energy efficient that takes only 25% of usable energy (Miskam et al., 2008). It has also further advantages like provision of all forms of energy, no net release of \( \text{CO}_2 \) and being very suitable for remote areas (Tewari et al., 2001). When carbonaceous materials are reacted with controlled amount of air/oxygen/steam at an elevated temperature and pressure from atmospheric to 2.4 MPa forms CO and H\(_2\) as the main product, the gas called syngas (Atnaw et al., 2011). The stoichiometric equation of the gasification process is (Inayat et al., 2010):

\[
\text{CF} + \text{LA} = \text{O} + \text{H}_2 + \text{CH}_4 + \text{CO} + \text{H}_2\text{O} + \text{N}_2
\] (1)

where, CF and LA stand for carbonaceous fuel and gasifying medium at lower than required for stoichiometric combustion.

Gas composition of syngas varies depending on the feedstock, particle size, gas and feedstock flow rate, chemical reactor configuration, operating conditions or the gasification process, gasifying agent and catalyst and gas residence time (Francisco et al., 2010; Inayat et al., 2010). This gas can be used as a standalone or duel fuel for power production or as an intermediate product for the production of synthetic natural gas, synthetic liquid petroleum, ammonia and methanol. Its energy density is very small compared to natural gas with Lower Heating Value (LHV) ranging between 4-6 MJ Nm\(^{-3}\) (Francisco et al., 2010). The LHV can be brought up in to the range of 9-13 MJ Nm\(^{-3}\) by using oxygen or steam for the gasification process (Fessum and Beyer, 1998). The production and utilization of syngas has 200 years long history and its milestones and historical terminologies are detailed in the literature (Richards and Casleton, 2010). Detail studies of syngas as a dual fuel in compression ignited engine, diesel as a pilot fuel and as a single fuel in a naturally aspirated SI engines are found in the literature. Even though the prospect of fuelling naturally aspirated spark ignition engine with syngas is very promising and even cost competitive with that of natural gas, it is associated with power de-rating that is mainly provoked by the decrease in volumetric efficiency (Dasappa et al., 2004; Sridhar, 2008; Sridhar et al., 2001). One way of enhancing this power de-rating is by the application of direct injection, filling the gas to a high pressure container. In this study, combustion features of syngas like energy density, laminar flame velocity and flammability limits of syngas are reviewed in detail and their effects on the combustion in a spark ignition engine are evaluated.

**GAS COMPOSITION AND CALORIFIC VALUE**

Depending on the feedstock, particle size, gas and feedstock flow rate, chemical reactor configuration, operating conditions or the gasification process, gasifying agent and catalyst and gas residence time, the gasification products also broadly vary. For a typical air blown gasification of a solid fuel, the major combustible products from the gasification are \( \text{H}_2 \), \( \text{CO} \), \( \text{CH}_4 \) and insignificant amount of heavy hydrocarbons that amounts around 50% of the total volume. This is diluted by the other 50% non combustible gases namely \( \text{N}_2 \) and \( \text{CO}_2 \). These gases are called lower calorific value gases and their LHV is in the range of 4-6 MJ Nm\(^{-3}\). When the gasification receives oxygen or steam instead of air, the amount of inert gases in the gasification product will be insignificant and the gas will be called medium calorific value gas (Hassan et al., 2010). The LHV for the gaseous
fuels is calculated by the summation of the partial LHV of each individual combustible gas component in the mixture (Fossum and Beyer, 1998), mathematically expressed as:

\[ \text{LHV} = \sum Y_i \text{LHV}_i \]  

where, \( Y_i \): Volume fraction of combustible gas component and \( \text{LHV}_i \): LHV of combustible gas component.

For a typical syngas with compositions of \( \text{H}_2: 10\% \), CO: 16\%, \( \text{CH}_4 \): 4, \( \text{N}_2 \): 53\% and \( \text{CO}_2 \): 17\%, the LHV calculated based on Eq. 2 is 4.508 MJ Nm\(^{-3}\). It might be assumed that there would be high power de-rating with the application of LHV syngas as a fuel for IC engine. However, engine performance is mainly based on the air-fuel mixture energy density and as a result; the engine power penalty is very small. Therefore, these gases are their application as a fuel has become increasingly important.

LAMINAR FLAME VELOCITY

The Laminar Flame Velocity (LFV) is the rate at which the flame propagates through quiescent unburned fuel-oxidant mixtures in the direction perpendicular to the expansion wave surface under laminar flow condition (Fossum and Beyer, 1998; Kuchta, 1985). As it is very sensitive to fuel-oxidant mixtures, LFV is a very essential parameter for the investigation of combustion chamber operation and emissions formation (Dam et al., 2010; Sridhar and Yarasu, 2010). It is influenced by the fuel composition, mixture equivalence ratio, temperature and pressure (Turns, 2000). Detail knowledge of laminar burning velocity or LFV and its influencing factors is mandatory in the study of Internal Combustion (IC) engines (Rallis and Garforth, 1980). At pressures and temperatures typical of unburned mixture, the LFV is measured experimentally in spherical closed vessels, by measuring cone angle in Bunsen burners and flame in the tube (Dam et al., 2010). As far as for pure combustible gases and single component fuels are concerned, there are adequately many literatures on the study of LFV (Monteiro et al., 2010).

Table 1 shows pure combustible gas’s LFV. However, compared to the importance of syngas in the energy sector and its complex mixture composition characteristic features, studies of laminar flame velocity are very insignificant. The study can be mainly categorized into \( \text{H}_2/\text{CO} \) mixture and on typical products of gasification with the proportion five of the constituent gases varied. As far as \( \text{H}_2/\text{CO} \) mixture is concerned again, many articles have been published (Bouvet et al., 2011; Burbano et al., 2011; Dam et al., 2010; Natarajan and Seitzman, 2010). LFV increased with an increase in \( \text{H}_2/\text{CO} \) ratio of mixture (Natarajan and Seitzman, 2010). With the later one on the other hand, the effect of inert diluent gases on the LFV is another interest. A detail literature survey has been conducted on the studies of LFV of syngas with an emphasis on the effects of fuel composition and its air-fuel ratio, temperature and pressure.

<table>
<thead>
<tr>
<th>Component</th>
<th>LHV (MJ Nm(^{-3}))</th>
<th>LFV (cm sec(^{-1}))</th>
<th>Flammability limit (% fuel in air)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>12.6</td>
<td>28.5</td>
<td>12.5-74.2</td>
</tr>
<tr>
<td>( \text{H}_2 )</td>
<td>10.7</td>
<td>210.0</td>
<td>4.0-74.2</td>
</tr>
<tr>
<td>( \text{CH}_4 )</td>
<td>35.8</td>
<td>40.0</td>
<td>5.0-15.0</td>
</tr>
<tr>
<td>( \text{O}_2 \text{H}_2 )</td>
<td>90-93</td>
<td>44.0</td>
<td>2.1-10.1</td>
</tr>
<tr>
<td>( \text{C}_2 \text{H}_6 )</td>
<td>56.3</td>
<td>67.0</td>
<td>2.7-36.0</td>
</tr>
</tbody>
</table>

Kishore et al. (2008) have numerically modeled the effect of hydrogen and diluents gas content of syngas on the LFV and stability of an outwardly propagating spherical flame. Both RUN1DL and PREMIX codes were employed in this investigation. On the zero stretch LFV, it was reported that the LFV increased with an increase in hydrogen at any equivalence ratio. This has indicated that the LFV was strongly influenced by the hydrogen content in the syngas. On the other hand, the presence of inert incombustible gases in the mixture severely affects the LFV. These gases reduce the reaction rate of the mixture and thus reduce the LFV (Natarajan, 2008; Natarajan and Seitzman, 2010).

When it comes to the effect of air-fuel ratio on the LFV of syngas, most of the literatures agreed up on its pick value at slightly fuel rich mixture around the stoichiometric. There is huge gap however with its pick value, particularly on the comparison of highest value of LFV of syngas and methane. For a typical syngas of 20% H₂, 20% CO, 2% CH₄ and the rest inert gases Sridhar et al. (2005) have reported that the LFV to be 50 cm sec⁻¹ at atmospheric condition and equivalent ratio (ϕ) of 1.0 which is 30% higher when compared to natural gas, Table 2. Similar to this, Liu et al. (2010b) have determined the LFV of a model syngas of 21% H₂, 24% CO and 51% N₂ as a function of ϕ. At an ϕ of 1.1, the LFV value is found to be around 50 cm sec⁻¹, in line with the previous study. On the other hand, Ouimette and Seers (2009) have compared the LFV of a typical syngas with LHV= 8 MJ Nm⁻³ with that of methane at initial pressure ranging from 0.1-1.52 MPa, temperature from 300-850 K and ϕ from 0.5-1.2. It was found to be lower than that of methane in all ϕ and even more pronounced at stoichiometric which was reported to be 37.5-20.2 cm sec⁻¹ for methane and syngas, respectively at initial conditions of 300 K and 0.1 MPa. Fossum and Beyer (1998) have reported a similar result on their comparison of LFV of LHV gas (syngas), mixture of LHV gas and methane and pure methane, which are something different to what is reported by (Liu et al., 2010a; Sridhar et al., 2005).

Effect of pressure and initial temperature on the LFV of syngas was also studies by different authors. Natarajan and Seitzman (2010) have reported a reduction in flame speed with an increase in pressure. Monteiro et al. (2009) have also used three syngas of different proportions of constituent gases with an ϕ of 1.0 for the study of laminar flame characteristics. It was found to be influenced by pressure and temperature and decreased with an increase in pressure while increased with an increase in temperature. Another investigation on the effect of initial temperature on the LFV was conducted by increasing the initial temperature from 300-850 K at an initial pressure of 0.1 MPa over a range of ϕ’s. The stoichiometric LFV increased from 37-270 cm sec⁻¹ and from 20-270 cm sec⁻¹ for methane-air mixture and syngas-air mixture, respectively. Sharp increase of LFV with an increase in an initial temperature was observed with syngas-air mixture compared

<table>
<thead>
<tr>
<th>Fuel-air mixture</th>
<th>H₂</th>
<th>CO</th>
<th>CH₄</th>
<th>Syngas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air/fuel ratio at ϕ = 1.0 mass</td>
<td>34.4</td>
<td>2.46</td>
<td>17.2</td>
<td>1.35</td>
</tr>
<tr>
<td>Mixture (MJ kg⁻¹)</td>
<td>3.41</td>
<td>2.92</td>
<td>2.76</td>
<td>2.12</td>
</tr>
<tr>
<td>Mixture (MJ Nm⁻³)</td>
<td>3.2</td>
<td>3.8</td>
<td>3.4</td>
<td>2.6</td>
</tr>
<tr>
<td>S_l limit (cm sec⁻¹)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lean</td>
<td>62</td>
<td>12</td>
<td>2.5</td>
<td>10.3</td>
</tr>
<tr>
<td>Rich</td>
<td>75</td>
<td>23</td>
<td>14</td>
<td>12</td>
</tr>
<tr>
<td>S_l at ϕ = 1.0 (cm sec⁻¹)</td>
<td>270</td>
<td>45</td>
<td>35</td>
<td>60</td>
</tr>
<tr>
<td>Peak flame temperature</td>
<td>2400</td>
<td>2400</td>
<td>2210</td>
<td>1800</td>
</tr>
<tr>
<td>Product/reactant mole ratio</td>
<td>0.67</td>
<td>0.67</td>
<td>1.00</td>
<td>0.87</td>
</tr>
</tbody>
</table>
to methane-air mixture. Similarly investigation of the effect of initial pressure on the LFV over the range of $\phi$ was conducted by increasing the initial pressure from 0.1-1.52 MPa at an initial temperature of 300 K. It has been reported that an increase in the LFV of both fuels was approximately proportional to $p^{0.2}$ and the stoichiometric value decreased from 37.10.5 cm sec$^{-1}$ and 20-6 cm sec$^{-1}$ for methane-air mixture and syngas-air mixture, respectively. It was also observed that the LFV was more sensitive to pressure at lean mixtures. The increase in LFV with an increase in initial temperature is attributed to an increase in reaction zone temperature, increase in thermal diffusivity and decrease of unburned mixture density (Natarajan and Seitzman, 2010; Natarajan, 2008).

On the prediction of performance of an IC engine fuelled by producer gas, Tinsut et al. (2006) have used the following correlation to determine the LFV of a typical producer gas:

$$S_k = S_{k,ref} \left( \frac{T_k}{T_{k,ref}} \right)^{0.2} \left( \frac{P_k}{P_{k,ref}} \right)^{0.1}$$  \hspace{1cm} (3)

where, $T_{k,ref} = 298$ K and $P_{k,ref} = 1$ atm.

The reference laminar flame speed is calculated from the following expression:

$$S_{k,ref} = B_{k} + B_{2} [P_{k} P_{ad}]^{0.25}$$  \hspace{1cm} (4)

The value of these constants $B_{k}$, $B_{2}$ and $F_{M}$ depend on the fuel type and composition.

**FLAMMABILITY LIMITS**

Another very important combustion parameter of the fuel, the flammability limit, is dependent on the composition of the mixture gases, hydrogen in particular. It defines the range of concentration of the fuel in a fuel-air mixture at a specified temperature and pressure that allows ignition initiated flame to propagate and sustain. It is mainly affected by the nature of the fuel, direction of the propagation, size and shape of the combustion chamber, temperature and pressure (Kuchta, 1985). He has developed a three dimensional flammability concentration-temperature-pressure diagram to show the effects of both temperature and pressure on the flammability concentration limit. The flammability limit is bounded by the upper (UFL) and Lower Flammability Limits (LFL) that indicate the maximum and minimum fuel concentrations in the fuel-air mixture, respectively (Fossum and Beyer, 1998). A flammability limit for a gas mixture is obtained from experiment (Heywood, 1988; Fossum and Beyer, 1998). It can also be calculated with the help of Le Chatelier's law with the following equation (Bjerketvedt et al., 1997; Hristova and Tchaoushev, 2006):

$$LFL_{mix} = \frac{100}{C_{1}/LFL_{1} + C_{2}/LFL_{2} + \ldots + C_{i}/LFL_{i}}$$  \hspace{1cm} (5)

where, $LFL_{mix}$ the lower flammability limit of the mixture $LFL_{1}$, $LFL_{2}$, ...$LFL_{i}$ the lower flammability limit of the constituent gases. The UFL and LFL of the some combustible pure gases are tabulated in Table 1.

$C_1, C_2, \ldots, C_i$ [vol. %] is the proportion of each gas in the fuel mixture without air.
Fig. 1: Flammability limits of H₂, CO and CH₄ containing varying range of N₂ and CO₂ (Coward and Jones, 1952)

The fact that hydrogen and carbon monoxide are the main flammable constituents of syngas, syngas inherits the characteristic features of these gases. However, the presence of inert gases in the gas mixture narrows the flammability limit. Coward and Jones (1952) have modified the Le Chatelier's law by including the effect of inert gases on the gas mixture flammability limit. In order to apply Le Chatelier's law for the gas mixture containing nitrogen and carbon dioxide, the mixture is first to be cut apart randomly in to simpler mixtures each containing only one combustible gas and one or all of the inert gases. The flammability limit of these simple mixtures is then to be read from the curve in Fig. 1. The flammability limit of gas mixture containing inert gases is then calculated by the modified Le Chatelier's law:

\[
\text{FL}_{\text{mix}} = \frac{100}{C_1/\text{FL}_1 + C_2/\text{FL}_2 + \ldots + C_i/\text{FL}_i}
\]

where, \(\text{FL}_{\text{mix}}\) the flammability limit of the mixture containing inert gases \(\text{FL}_1, \text{FL}_2, \ldots, \text{FL}_i\) the flammability limit of the dissected mixtures, read from Fig. 1.

\(C_1, C_2, \ldots, C_i\) [vol.%] is the proportion of each dissected gas in the mixture without air (Coward and Jones, 1952).

Fossum and Beyer (1998) estimated the flammability limit of a typical syngas in the range of 20-60% fuel in air. For a typical syngas with compositions of H₂: 10%, CO: 16%, CH₄: 4, N₂: 53% and CO₂: 17%, the flammability limit based on Eq. 6 is calculated and the random dissection of the constituent gases is depicted in Table 3.

Substituting the LFL and UFL values in Eq. 5 along with the total mixture proportion gives:

\[
\text{LFL}_\text{syn} = 24.1\% \text{ volume fuel in air}
\]

On the same manner:

\[
\text{UFL}_\text{syn} = 59.92\% \text{ volume fuel in air}
\]
This range (24.1-59.92% volume fuel in air) is very wide although, the lower flammability limit is bigger compared to compressed natural gas and gasoline of upper and lower flammability limits of 5-15 and 1.4-7.6%, respectively. Flammability limit, the lower flammability limit in particular, is indicator of combustibility of fuels (Chomiak et al., 1989) and therefore more emphasis should be given to the engine atmosphere, oxidizer (air-fuel ratio) and ignition energy for the sustainability of combustion. Flammability limit is a very important characteristic in the safety and fuel for IC engine research.

**DISCUSSION**

LHV of syngas mainly depends on the volume percentage of the combustible constituent gases in the mixture. Among these, methane takes the lion’s share. The range of LHV of a typical syngas, constituting more than 50% non combustible inert gases (CO₂ and N₂) in the mixture, is from 4-6 MJ Nm⁻³ compared 35.8 MJ Nm⁻³ of CNG. CNG is a conventional gaseous fuel for IC engines and mostly comparison is made with CNG. One may think that there is a comparative reduction in the power output when syngas is applied in IC engine. However, as can be seen from Table 2, the difference in in-cylinder charge mixture’s heating value of syngas and CH₄ is very small (Sridhar and Yarasu, 2010). In addition to this, the power de-rating can be further narrowed down by increasing cylinder compression ratio and by the application of direct injection system. In direct injection engine, there is low fuel consumption because of reduced pumping losses and heat transfer losses (Cho and He, 2007) and the volumetric efficiency penalty will be minimal. However, it is worth to note the high disparity of stoichiometric air-fuel ratio of syngas and CNG, 1.35-17.2, respectively. This fact demands high flow rate injection of syngas in to the cylinder almost 1 m³ of fuel for a 1.35 m³ of air. This will be a huge challenge in the injection strategy as it requires higher injection duration in contrary to the late injection aimed to improve the volumetric efficiency of the engine.

The variability of fuel composition of syngas is the major challenge in the investigation of LFV in addition to the other variables like pressure and initial temperature. Understanding the LFV of syngas is very critical for the understanding of the combustion behavior in an IC engine. The main combustible gases that construct syngas are H₂ and CO. As can be seen from Table 1, the LFV of H₂ at stoichiometric and atmospheric condition is around 210 cm sec⁻¹. An increase in concentration of H₂ in the mixture increases the overall reactivity and as a result, the concentration of H₂ in the
mixture significantly influences the mixture LFV. As far as the third combustible gas, CH₄ is concerned, its concentration in the mixture is very minimal and its effect on the LFV of the reactant mixture is insignificant. The non combustible inert gases on the other hand affect both the reaction rate and adiabatic flame temperature of the reactant mixture. As the result the LFV of the reactant mixture decreases with an increase of concentration of diluents in the mixture.

Air-fuel ratio of the reacting mixture is also one major variable that significantly affect the LFV of syngas. There is a general agreement with all the previous works over the air-fuel ratio for the maximum laminar flame speed value. However, there is lack of consistency with the value. While some place the value in the range of 45-50 cm sec⁻¹ which is higher than that of LFV of CNG (35-40 cm sec⁻¹), others put it in the range of 20 cm sec⁻¹. In fact we shouldn’t put aside the effect of composition variation of the mixture. But LFV of syngas and its influencing variables should have to be further investigated systematically with an emphasis on the IC engine operation conditions.

The mixture in a direct injection spark injection engine or any premixed combustion engine like gas turbine combustion is not homogeneous. The atomization takes place in the combustion chamber just prior to ignition. With this setup, there will be a local mixture where flame will not be able to properly propagate. With this regard, flammability limit, the LFL in particular is very important parameter. There is limited experimental work with regard to the flammability limit of syngas, in contrary to the pure combustible gases. The presence of diluent gases in the fuel mixture narrows the flammability limit. Most articles estimated the flammability limit of syngas in the range of 20-60% fuel in air. The LFL of syngas is higher compared to CNG and gasoline, 5 and 1.4% fuel in air, respectively. As a result, combustion of syngas needs stronger ignition source, high compression ratio and high temperature environment to bring down the LFL.

CONCLUSIONS

In this study, we have found that the low calorific value of syngas has little effect on the power output when compared to CNG. Furthermore, the power de-rating can be further minimized with the application of direct injection in a higher compression ratio engine. Both laminar flame speed and flammability limit, lower flammability limit in particular, have been found very important combustion parameters in premixed combustion. However, there is lack of consistency in the literature with the value of laminar flame speed of syngas. With this regard, application of existing results of laminar flame speed for the combustion modeling in high compression ratio, high temperature engine environment is very difficult. Further background study of both laminar flame speed and flammability limit of syngas in this specific environment is quite critical both experimentally and numerically.

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REFERENCES


