CFD Simulation of Producer Gas Fuelled SI Engine

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Abstract. Syngas generated from the thermochemical conversion of biomass in a gasifier is increasingly being used for fuelling internal combustion engines, especially for distributed power generation. Producer gas as a fuel has thermo physical properties significantly different from those of conventional fuels. As of date, there are no dedicated engines for alternative fuels in general and producer gas in particular. A review of the available literature indicates experimental experience with producer gas but very little information on modelling and simulation studies are available. While experimental investigations provide actual performance parameters, the information is essentially spatial or temporal average only. Apart from that, fluid dynamic and combustion progress parameters cannot be acquired inexpensively. The current work primarily addresses the combustion progression parameters in a typical spark ignited engine under naturally aspirated and turbocharged after cooled configuration at varying mixture quality using the ANSYS FLUENT computational fluid dynamics software. The CHEMKIN software is used for determining the laminar flame speed for producer gas as a function of the mixture quality. Spatially averaged pressure traces from the simulation are compared with literature pressure traces at the desired condition and various simulation parameters are tuned till a match between the literature and simulation pressure is obtained. Once the simulation is validated, the progress of combustion parameters is derived from the simulation in post processing.

Keywords: Producer gas, Laminar flame speed, CHEMKIN, IC engine, CFD simulation.

1. Introduction
In the current scenario, all the energy conversation devices have been fuelled with hydrocarbon based fuels formed over millions of years. Country like India which completely depends on the import of the hydrocarbon based fuels. According to the estimates oil peak have been already been surpassed, in feature oil importing countries like India are expected to worst hit due to the major dependence on the import of the hydrocarbon based fuel. Increase in the hydrocarbon based fuels is in one of the major reason for atmospheric pollution and the drastic changes in the weather pattern are being attributed to the large amounts of CO₂ released by the combustion of hydrocarbon fuels [1]. Currently to address the above mention twin challenges various studies have been carried out by research teams across the globe. Renewable energy sources will play an important role in address the issues related to the fossil fuels. Renewable energy has the potential to provide zero emission of pollutants, also it can address the meet the small scale and rural needs like decentralized power system in a reliable and environmentally sustainable way. Is as been estimated that by 2040 renewable sources will contribute 47.7% of the total global energy requirement [2] [3].
Biomass is one of the alternative fuel to replace the conventional hydrocarbon based fuels and also addressed environmental concerns the fact that with bio derived fuels retention time of CO\textsubscript{2} in the atmosphere is much lower than the time required for CO\textsubscript{2} to start contributing to global warming. Biomass can be broadly based on the moisture and lignin content, those with less lignin (less than 10%) and high moisture beyond 70% can be used for bacterial conversion processes – the processes of biological conversion root when largely yields in the gas consisting of CH\textsubscript{4} and CO\textsubscript{2}. Biomass with high lignin (more than 10%) with reasonable less moisture (less than 30%) can be used for thermo-chemical conversion processes which yields gas known as synthetic gas or commonly known as syngas. Syngas basically consists of H\textsubscript{2} and CO and some trace of methane as combustible species [4] [5].

Producer gas (PG), a bio-derivative alternative gaseous fuel generated from thermo-chemical conversion of biomass. Producer gas typical composition of 20% CO and H\textsubscript{2}, 2% CH\textsubscript{4} and balance incombustibles has thermo-physical properties significantly different from standard gaseous fuels as highlighted in table 1. The comparison of the PG with CNG is more vital because CNG is considered as one of the standard gas fuels with regards to commercial availability of thermal conversion devices like IC engine, industrial burners etc., which can be easily be modified for the other gas fuel operations [6]. The difference in the thermo-physical properties would potentially require study of certain fuel specific features. The air fuel ratio of the PG gas is about 1.30 compared to that of Natural gas (CNG) is 17.0 on mass bases which differ in terms of magnitude when compared to CNG. In the same line PG calorific value also varies in the ratio of 1:10 when compared to that of CNG gas. Laminar flame speed for PG is 20% higher compared to that of the CNG. Even though the calorific value of the PG is very less when compared to CNG the mixture caloric value is less by 23%. The adiabatic flame temperature (AFT) are also lower for PG when compared to CNG and Hydrogen [7].

| Fuel Property                  | H\textsubscript{2} | CNG  | Bio-gas | PG   |
|-------------------------------|---------------------|------|---------|------|
| Air to Fuel (kg/kg)           | 34.4                | 17.0 | 10.5    | 1.30 |
| Calorific Value (MJ/kg) at \(\phi = 1\) | 121.0              | 50.0 | 23.6    | 5.0  |
| Laminar flame speed (m/s) at \(\phi = 1\) | 2.70               | 0.40 | 0.26    | 0.50 |
| Mixture LCV (MJ/kg) at \(\phi = 1\) | 3.41               | 2.78 | 2.30    | 2.17 |
| Adiabatic Flame Temperature (K) at \(\phi = 1\) | 2360               | 2214 | 2102    | 1873 |

Literature survey in the field of producer gas can classified into generation and its application. Generation of producer gas has been reported since World War II, European nations which as exploited the gasification technology during the World War II because of the petroleum oil crisis. National Swedish Testing Institute of Agriculture Machinery, Sweden has reported work on the design and development of closed top gasification systems [8]. In the recant time Indian institute of Science, Bangalore has worked on open top downdraft gasification technology, which is able to generate the engine quality producer gas with low contaminate and also gasifier is able to handle any solid biomass with moisture content less than 20% [9]. In the contest of producer gas application, Dasappa et al have reported major factors influencing the power output of the diesel frame engine converted to operate on producer gas, also presented some actual field studies [10]. Sridhar et al as reported experimental study of SI engine operated for high possible compression ratio to establish the engine performance, he has also reported the performance analysis of small and medium scale engine derived from diesel frame converted for producer gas operation by replacing spark plug in the place of fuel injector [9]. Shivapuji et al reported the experimental and quasi dimensional analysis of multi-cylinder SI engine operated on producer gas operated in both natural aspirated and turbocharge mode to establish the peak load operation [11]. Biomass to electricity efficiency has been reported to be at 18% for naturally aspirated mode which increases to 22% under turbocharged mode of operation. Emissions under both the modes of operation are reported to be well within the international permissible limits [12] [13]. Yarasu et al has reported on the turbulent combustion of producer gas in closed vessels and engine cylinders. The main objective the work has been multi-dimensional simulation of turbulent combustion in the bowl-in-piston
engine operating on producer gas fuel and to observe the flame and flow field interaction [14]. Ulugbek Azimov et al has reported on a CFD simulation of syngas fuelled turbocharged duel fuel system. The modelled results were validated by comparing predictions against corresponding experimental data for a supercharged dual-fuel engine [15].

A review of the available literature on experimental and simulation studies indicates that which significant amount of experimental work has been done covering a broad range of aspects dealing with producer gas fuelled operation, the modelling and simulation has largely been restricted to zero and quasi dimensional studies. No significant work is reported on full 2D computational fluid dynamics simulation. The motivation for the current work stems from this lack of availability of information in the 2D CFD simulation area which is sought to be addressed over the full cycle of a four stroke cycle on fuelling with producer gas. the scope of the current work spans obtaining the geometric specifications of the engine of interest, modelling the 2D geometry, deriving the 2D mesh using appropriate scheme, arriving at the initial and boundary conditions, establishing of laminar flame speed correlations as a function of engine operating parameters; primarily the equivalence ratio and finally the full simulation of the engine for peak load conditions. The simulation results are validated using literature data from reported on the in-cylinder investigation of a multi-cylinder engine fuelled with producer gas by Shivapuji et al. Post the validation, spatial analysis of various parameters of interest related progress of combustion are extracted from the simulation in post processing exercise and reported.

2. Multi-dimensional model formulation

Conservation equation formulation

The modelling approach in based on the unsteady Reynolds Average Navier-Stokes (RANS) to solve the mass and momentum conservation equations. Mass and momentum equation are solved together for the proper calculation of pressure gradient in the momentum equation. Also energy conservation equation is solving to account of the energy conservation in the system. The compressible mass and momentum equation are given as follows,

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i
\]

In the above equation, \(\rho\) is fluid density term, \(u\) is velocity term, \(P\) is pressure term, \(\sigma_{ij}\) is viscous stress tensor, and \(S\) is the source term. Redlich-Kwong equation is used to couple density pressure and temperature terms for solving compressible mass and momentum equation [16].

\[
\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_j} = -P \frac{\partial u_i}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \rho D m h_m \frac{\partial Y_m}{\partial x_j} \right) + S
\]

Where, \(\rho\) is density, \(P\) is the pressure, \(D\) is the mass diffusion, \(Y_m\) is the mass fraction of species \(m\), coefficient, \(e\) is the specific internal energy, \(K\) is the conductivity, \(hm\) is the species enthalpy, \(\sigma_{ij}\) is the stress tensor, \(S\) is the source term and \(T\) is temperature. Transport equation describing conservation of chemical species consisting of convection, diffusion and chemical reaction source for each component of species is solved [16]. Where \(c\) is the chemical concentration of the species, \(D\) is the diffusion coefficient and \(S\) is source term.

\[
\frac{\partial c}{\partial t} + \frac{\partial u c}{\partial x_j} = \frac{\partial}{\partial x_i} \left( D \frac{\partial c}{\partial x_i} \right) + S
\]

Combustion formulation

The flame may be freely propagating as it when flame is initiated in a tube containing combustible gas mixture. Laminar flame speed is function of pressure and temperature for given equivalence ratio, the
flame approaches the unburned mixture at laminar speed, $S_L$. The unburned gas enters the flame in a
direction normal to the flame sheet. Since the heat heats the products, the burnt density is less than the
unburned density. Continuity thus requires that the burned gas velocity is higher than the unburned gas.
The flame consists of two regions they are the preheat zone and reaction zone In preheat zone where
little heat is released, the temperature of unburned gas is raised mainly due to the conduction from the
reaction zone and the reaction zone where the bulk of the chemical energy is released in the form of heat
results in the zone. The region between the temperature where exothermic chemical reaction begins and
the hot boundary at the downstream equilibrium burned gas temperature is called the reaction zone. The
thickness of preheat zone can be calculated for one dimensional flames from conservation equations of
mass and energy [16]. The thickness of the preheat zone $\delta_L$ is

$$\delta_L = \frac{4.6 k}{c_p \rho_u S_L}$$  \hspace{1cm} (5)

The laminar flame speed at pressure and temperature typical of unburned mixture in engines are usually
measured in spherical closed vessels by propagating a laminar flame radially outside from vessel centre
[16]. The laminar speed is then given by

$$S_L = \frac{d m_b}{A_f \rho_u}$$  \hspace{1cm} (6)

Where the mass rate is determined from the rate of pressure rise in the vessel and the $A_f$ is the flame
area.

Metghalchi and Keck experimentally determined the laminar flame speed for various fuels over a range
of temperature and pressure typical conditions associated with the internal combustion engines. The
laminar flame speed for different fuel-air mixture have fitted by simple power law [17].

$$S_L = S_{L,ref} \left( \frac{T_u}{T_{u,ref}} \right)^{\alpha} \left( \frac{P}{P_{ref}} \right)^{\beta} \left( 1 - 2.1 * Y_{dil} \right)$$  \hspace{1cm} (7)

Where $T_{u,ref} = 298K$ and $P_{ref} = 1atm$ are the reference temperature and pressure, $S_{L,ref}$, $\alpha$ and $\beta$ are the
constants for given fuel, equivalence ratio, and burned gas diluent fraction the term $Y_{dil}$ is the mass
fraction of diluent present in the air-fuel mixture [12][13]. For Methane, propane, isoctane and methanol these constants can be represented as follows,

$$S_{L,ref} = B_M + B_2(Fr - FM)^2$$  \hspace{1cm} (8)

Where $B_M$, $B_2$ and FM are constants depending upon the fuel type. The temperature and pressure
depends on the value of $\alpha$ and $\beta$ which are the function of equivalence ratio (Fr), expressed as follows

$$\alpha = 2.18 - 0.8(Fr - 1)$$  \hspace{1cm} (9)

$$\beta = -0.16 + 0.22(Fr - 1)$$  \hspace{1cm} (10)

The reference laminar flame speed is calculated using the equation 8, for different equivalence ratio $\alpha$
and $\beta$ values are calculated using equation 9 and 10. By knowing $S_{L,ref}$, initial pressure and temperature
Laminar flame speed ($S_L$) can be calculated from equation (8). Analysis by Damkohler also known as
the Damkohler paradigm, puts the turbulent combustion within a spark ignited (SI) engine in the
wrinkled laminar flame (flamelet) regime. In this regime, the cylinder content is divided into burned and
unburned regions separated by an infinitesimally thin but highly wrinkled reacting flame sheet. This thin
sheet is basically the laminar flame sheet with flame thickness ($\delta_L$) less than the regime for the
Kolmogorov micro-scale. In the flamelet regime, a reaction progress variable ‘c’ having a value between
0 (unburned mixture) and 1 (burned gas) describes the progress of combustion and is described as in
equation 11 where ‘n’ is the number of products, Yi is the mass fraction and $Y_{i,eq}$ is the equilibrium mass
fraction of the i$^{th}$ specie [18].
\[ c = \frac{\sum_{i=1}^{n} Y_i}{\sum_{i=1}^{n} Y_{eq}} \]  

(11)

In ANSYS FLUENT, the flame front propagation is modelled by solving the transport equation where \( S_c \) and \( S_e \) represents the turbulent Schmidt number and the reaction progress source term respectively as presented in equation 12.

\[
\frac{\delta (\rho c)}{\delta t} + \nabla \cdot (\rho \bar{v} c) = \nabla \left( \frac{\mu_t}{S_c} \nabla c \right) + \rho S_c
\]

(12)

The mean reaction rate in the above equation ‘\( \rho S_c \)’ is modelled along the Zimont model and is given by equation 13 where \( \rho_u \) and \( U_t \) stand for the density of the unburned mixture and the turbulent flame speed respectively.

\[ \rho S_c = \rho_u U_t |\nabla c| \]  

(13)

The turbulent flame speed \( U_t \) is modelled considering the highly wrinkled and thickened front as in equation 14 below where, \( u' \) the root mean square velocity, \( U_l \) the laminar flame speed, \( \alpha \) the thermal diffusivity and \( l_t \) the turbulent scale [18].

\[ U_t = A (u')^{3/4} U_l^{1/2} \alpha^{-1/4} l_t^{1/4} \]  

(14)

3. Simulation methodology

Initially laminar flame speed was calculated using the CHEMKIN simulation software for different initial pressure and temperature and by least square fits the constants were determined for the equivalence ratio when are necessary inputs for the engine combustion simulation in ANSYS-Fluent. The determined laminar flame speed values were compared against the available literature data. Once the laminar flame speed constants values are in expectable error band width i.e is within 2 to 3% the values \( \alpha \) and \( \beta \) were used in the engine combustion simulation.

Main prerequisite for CFD simulation is the geometry modelling and discretization of the fluid domain. In the current work engine geometry were modelled from the literature report by Shivapuji et al [19]. 2D model was created consisting of intake, exhaust and piston geometry was modelled and meshed in ICEM-CFD software. 2D simulation was chosen because it is of simple geometry, and take less time take for the simulation when compared with the time taken for 3D simulation, but it fails to capture the turbulence parameters. Once the mesh is created it is imported to ANSYS-FLUENT wherein the dynamic mesh was created i.e. moving boundary was created for intake, exhaust and piston parts and respective profile were assigned. After the creation of dynamic mesh the mesh is previewed to verify the mesh proper moment according to the profile assigned to different regions. The simulation initiated by assigning initial values for the variable, namely initial pressure, temperature. The fuel properties such as laminar flame speed un-burnt fuel mass fraction, lower calorific value of fuel and spark timing are also assigned.

Simulation was carried out initially to validate the literature data and then parametric of load variation was carried out for natural aspirated and turbocharged mode conditions. In all the cases the laminar flame speed coefficients were same, laminar flame speed coefficients were defined using User defined functions (UDF) in ANSYS-FLUENT interface. Unburnt fuel fractions were calculated based on the operating equivalence ratio and defined in the ANSYS-FLUENT. Initial pressure, temperature were defined based on the simulation load conditions.

4. Results and Discussion

Laminar flame speed coefficients calculation

CHEMKIN results for estimation of laminar flame speed for different initial pressure and temperature and by least square fits the constants were determined for the equivalence ratio of the range 0.8 to 2.014,
Fig. 1 show the plot of laminar flame speed of producer gas determine using CHEMKIN for different equivalence ration (\(\Phi\)) for atmospheric conditions at 1 bar and 300 K, engine like conditions at 25.4 bar and 716 K. \(S_L\) Tinaut are the values from the literature [20] and \(S_L\) Chemkin are the values obtained from the CHEMKIN software. Laminar flame speed is high at the rich conditions.

![Figure 1. Laminar flame speed vs. equivalence ratio (\(\Phi\)).](chart1.png)

![Figure 2. Laminar flame speed for different inlet temperature at inlet pressure 1 bar.](chart2.png)

The variation of laminar flame speed for varies inlet temperature by maintaining the inlet pressure constant were calculated. It was observe the laminar flame speed at low pressure and high temperature the laminar flame speed is high. But the laminar flame speed goes on decreasing as one increases the inlet pressure and temperature. It can be observed that the laminar flame speed at 10bar and 900K inlet condition the laminar flame speed is about 2.2 m/sec. Fig.2and 3 show the plot of laminar flame speed for different inlet temperature at inlet pressure conditions 1 and 10 bar respectively and the obtained values are compared with the literature (Tinauts) values.
Figure 3. Laminar flame speed for different inlet temperature at inlet pressure 10bar.

Figure 4. Comparison between the CHEMKIN and literature values for different equivalence ratio.

Fig. 4 gives the comparison of laminar flame speed at different equivalence ratio for the values obtained from CHEMKIN and literature (Tinauts) values. In Table 2 shows the constants values obtained from least square fits methods the first row represent the values obtained from the CHEMKIN, and second row represents the from the literature.

Table 2. The details of the constants determined by using CHEMKIN and literature

| Fuel                  | FM       | BM           | B2             | α       | β       | $S_{L,ref}$ (m/sec) |
|-----------------------|----------|--------------|----------------|---------|---------|---------------------|
| Producer Gas (CHEMKIN)| 1.365    | 48.00e-02    | -150.00e-2     | 2.18    | -0.56   | 0.43                |
| Producer Gas (F.V.Tinaut)| 1.186    | 50.06e-2     | -82.70e-2      | 2.0     | -0.4    | 0.47                |
Validation of 2D CFD simulation result with literature data

2D simulation in-cylinder pressure – crank angle results for the peak load operation of the engine under naturally aspirated and turbocharged operation respectively. Literature reported was the experimental results represent the ensemble average of 250 consecutive cycles, near complete match of the traces can be observed with a small deviation observed during the expansion stroke for 2D simulation.

| Table 3. Comparison of magnitude for Experimental and Simulation |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Mode of operation               | Peak position (deg) | Peak value (bar) | Peak position (deg) | Peak values(bar) | Difference Peak value (%) |
| TA                              | 374              | 74.4            | 374              | 76.1            | 2.25             |
| NA                              | 375              | 34.4            | 374              | 34.0            | 1.17             |

Figure 5. Plot of Pressure-Crank angle for Literature and simulation values for NA mode.
Figure 6. Plot of Pressure-Crank angle for Literature and simulation values for TA mode.

The outcome of the experimental and 2D simulation results are consolidated in Table – 3, where the position and magnitude of peak pressure are compared for the literature and simulation results. It can be observed that the deviation in the peak pressure at is at around 2.25% for TA and 1.17% NA mode of operation respectively. The position of peak pressure differs by 1 degree which is well within the cyclic variability limits of engine operation.

5. Conclusion

In the current work, Laminar flame speed calculations using CHEMKIN package at various equivalence ratio, pressure and temperature are used to establish the expression for laminar flame speed as a function of equivalence ratio, pressure ratio and temperature ratio. Using the established expression for laminar flame speed, 2D simulations were developed for computational fluid dynamics model using the initial conditions and boundary conditions from Literature. Comparing literature and simulation cylinder average pressure indicate a very close match validating the computational fluid dynamics simulation. The simulations have been carried out considering the in-cylinder mixture as an ideal gas and in place of the chemical kinetics established expression for laminar flame speed was used as user defined functions. Overall 2D simulation were carried and achieved good match with the literature data within expectable error range of 2.5%.

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