# Sensitivity analysis of mixture quality on combustion phasing and its impact on 0D simulation of a producer gas fuelled multi-cylinder engine

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### Abstract

In-cylinder investigations of producer gas fuelled operation of a spark ignited engine at different loads and mixture quality are reported. The equivalence ratio operating regime is established based on the knock limit on the rich side and cyclic variations on the lean side. The impact of mixture quality on combustion phasing is reported. Combustion phasing is quantified based on the Wiebe shape factor at a fixed efficiency factor, established based on the exhaust thermal and chemical enthalpy. First law based 0D modeling approach is adopted for engine simulation with Wiebe function heat release. The Wiebe function, though fuel specific, remain broadly independent of the load. Sensitivity analysis of engine simulation towards combustion phasing indicates the possibility of using fuel specific coefficients to simulate a rather broad range of engine operating conditions, especially load and mixture quality. The deviations therein are within the limits of cyclic variability for producer gas fuelled operation.

## **1** Introduction

Combustion phasing in a spark ignited (SI) internal combustion (IC) engine is analytically quantified in terms of the shape and efficiency factors of a cumulative distribution function known as the Wiebe function [1][2]. The Wiebe function simulates the heat release in the engine in terms of fuel mass fraction burned as a function of the crank angle in a first law based 0D model. The accuracy of the 0D model thus depends on the values of the Wiebe coefficients. For typical hydrocarbon based conventional fuels (gasoline), a shape factor of 2 and efficiency factor of 5 has been established [3].

With the increasing use of alternative fuels to mitigate economic and environmental concerns [4], the choice of Wiebe coefficients for engine simulation is a critical issue. As the combustion phasing primarily depends on the fuel thermophysical properties [3] and with the properties of alternative fuels differing significantly from those of conventional fuels [5], a suitability assessment of coefficients for conventional fuels and if necessary establishing fuel specific coefficients become imperative. The present authors, in a previous work dealing with Producer Gas (PG), a bio-derived gaseous alternative fuel generated from the thermo-chemical conversion of biomass [6], have critically addressed the need for fuel specific Wiebe coefficients towards an accurate simulation. The authors have reported a load independent shape and efficiency factors of 1.7 and 2.4 respectively for a typical gas composition [7].

The focus of the current work is to address the sensitivity of combustion phasing to variations in the mixture quality and its impact on 0D simulation. The variation in the mixture quality could arise due to a change in the feed gas composition or due to controlled changes in the air-fuel ratio supplied to the engine. The combustion phasing is analyzed in terms of the cumulative heat release trace(s) derived from the in-cylinder pressure traces acquired on a PG fuelled engine over the extreme supported equivalence ratio range for different loads, under maximum brake torque (MBT) ignition settings. With the identification of specific shape factors, the sensitivity of the 0D simulations, specifically the magnitude and position of peak pressure, to operating condition specific and load average Wiebe coefficients is reported.

# 2 Methodology

Experimental investigations involved the operation of a six cylinder natural gas (NG) engine operated on PG under turbocharged after-cooled mode. In-cylinder pressure traces were acquired as a function of crank angle by means of a spark plug adapted pressure sensor. The MBT ignition timing is established by a spark sweep test and subsequently the engine is operated from no load to full load in approximate steps of 10 kWe. The peak supported load of 72.8 kWe on the engine is knock limited. At the four loads of 40 kWe, 50 kWe, 60 kWe and 70 kWe, the mixture quality is varied by changing the airfuel ratio between rich and lean conditions to establish the limiting mixture quality. It is observed that the rich and lean mixture quality limits at any load are limited by knock and cyclic variations respectively. The normal operating point is identified as the simultaneous minimum of engine cyclic variations and the specific gas consumption.

The acquired pressure trace(s) along with the cylinder volume change rate are used in the rate form of the first law of thermodynamics to get the cumulative heat release rate (HRR). The Wiebe efficiency factor, representing the fuel conversion efficiency in the engine is estimated based on exhaust temperature and composition measurement (representing chemical and thermal enthalpy). The Wiebe shape factor is established by means of an exponential least square curve fit approach. A first law based 0D model is developed wherein the gas exchange process is modeled along the filling and emptying technique while heat is considered to be exchanged between the cylinder (treated as the lumped mass) and the surrounding across a hypothetical boundary with no source term within the cylinder. The Wiebe function is used in the first law based 0D model to simulate the heat release in the engine.

## 3 Results and discussions

A spark sweep test towards establishing the MBT ignition timing for PG provides 22 deg before top dead center (bTDC) as the MBT timing against 28 deg for NG operation. The 6 deg retard is attributed to the nearly 40% higher flame speed for PG (~50 cm/s) as compared to NG (~35 cm/s). Figure 1 presents

the pressure crank angle traces at the top three load (restricted for brevity) with the outcome of the spark sweep test indicated as inset data. The peak supported load is 72.8 kWe, beyond which features indicative of incipient knock are observed. Such a distortion, after the peak pressure, is clearly visible on the 74 kWe pressure trace.



Figure 1. P-Theta at MBT and spark sweep test

At the loads of 40, 50, 60 and 70 kWe, the mixture quality was varied between rich and lean conditions to identify the limiting air-fuel ratio supported by the engine while maintaining the ignition timing at 22 deg bTDC. The investigation has revealed that the lean operation of the engine is limited by the cyclic variations while the rich operation is limited by end gas auto-ignition. On the lean operating, the permissible engine speed (alternator frequency) fluctuation band of 1485 rpm (49.5 Hz) and 1506 rpm (50.2) Hz (Indian standards) [9] was considered for establishing the limit. Figure 2a presents the engine speed response under steady and hunting operation (mixture quality beyond the lean limit) with the permissible band included while figure 2b presents characteristics of rich side knocking cycles.



Figure 2 (a) Speed variation (lean operation) and (b) Knocking cycles (rich operation).

While heavy knock is characterized by high frequency fluctuations on the cylinder pressure trace, in the current case incipient knock has been considered as the load and mixture quality limiting condition. Since incipient knock cannot be clearly detected on the pressure trace (refer figure 2b), the pressure signal is subjected to spectral analysis (Fast Fourier Transformation) as it has been established that, knock excites characteristics frequencies in the 5 kHz to 7 kHz range [3] and a presence of these frequencies in the spectrum indicates knock. The result of spectral analysis is shown in figure 3.



Figure 3. Spectral analysis of knocking cycles

Having established the limiting criteria, the extreme limit operating mixture quality is determined for four loads as shown in figure 4. The maximum error in the equivalence ratio is  $\pm$  2.5%. It can be observed that the normal operation regime, corresponding to the simultaneous minimum of specific fuel consumption and cyclic variations is on the overall rich side at an equivalence ratio of about 1.1 for all the loads. The lean limit of the peak load is also on the slightly richer side.



Figure 4. Mixture quality and load limited operating regime

The requirement of richer than stoichiometric mixture quality for normal engine operation is attributed to the PG flame speed peaking at richer than stoichiometric conditions. This is evident from figure 5 where the variation of the laminar flame speed estimated using the CHEMKIN package [8] as a function of equivalence ratio is presented. It can be observed that under both atmospheric and post compression engine like conditions for the unburned mixture, the flame speed peaks on the richer side.



Figure 5. Variation of laminar flame speed with mixture quality

The operating condition corresponding to the peak flame speed is significant considering that, due the small combustion duration, the cyclic variations are minimum and the degree of constant volume combustion is highest, giving higher fuel efficiencies. Due to the above cited reasons, the normal operating quality gets positioned on the richer side. As for the lean and rich operating limits, the tendency is to converge towards the normal operating conditions with an increase in the

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load. It can also be observed that the lean limit shows low sensitivity to the load as compared to the rich. Further, the lean and rich limits follow opposite trends and the operable mixture quality band narrows with an increase in the load. While a detailed discussion dealing with the above response is outside the scope of the current work, a brief argument is presented as below.

On the significant reduction of the rich limit (knock limited) with load, while an increase in the load leads to an increase in the in-cylinder temperature and turbulence, in turn increasing the flame speed, the impact of higher unburned temperature on the auto ignition time is far greater as compared to the increase in the flame speed. The only way of curtailing knock as the load increases is by reducing the concentration of the most reactive specie, in this case  $H_2$  [9]. Thus, with an increase in the load, a relative leaning of the mixture quality is required towards ensuring knock free operation.

The effect of mixture quality on the combustion phasing in terms of the cumulative heat release pattern is shown in figure 6 for PG fuelled operation under normal and extreme mixture quality limit operation of the engine at two loads of 40 (fig 6a) and 70 kWe (fig 6b) (restricted for brevity). The stoichiometric-MBT heat release pattern for gasoline is also presented.



Figure 6. Cumulative heat release pattern

When comparing the heat release pattern of PG with that of gasoline, it can be observed that the gasoline heat release profile differs significantly from PG heat release profiles for all the operating conditions. The details describing the differences and the factors causing the differences have been addressed by the authors elsewhere [7]. The present authors have reported a load independent shape factor of 1.7 for a typical PG composition of 14±0.5% CO, H<sub>2</sub> and 1.2±0.4% CH<sub>4</sub> with balance being incombustibles [7]. In the current work, for PG composition of  $18\pm0.5\%$  CO, H<sub>2</sub> and  $0.8\pm0.2\%$  CH<sub>4</sub> and balance incombustibles, the least square curve fit analysis indicates the shape factor to be 1.82 for the same efficiency factor of 2.4 over the 2 to 90% combustion range. The difference in the shape factor for two different compositions highlights the sensitivity of the combustion phasing and hence the shape factor to the fuel composition and energy density. The criticality of correct choice of the Wiebe coefficients can be gauged from figure 7 where failure of simulation is evident when an attempt is made to simulate PG fuelled operation using Wiebe coefficients tuned for conventional fuels.



Figure 7. Effect of improper choice of Wiebe coefficients

On the variation of the combustion phasing with mixture quality, it can be observed from figure 6 that the combustion duration for the normal operation is lower than both the rich and lean operation durations. At the peak load, the phasing for rich and normal operations nearly overlap with only a subtle difference due to the close positioning of the corresponding equivalence ratios (refer figure 4). For normal engine operation, the higher flame speed as compared to the extreme limit operating conditions reduced the combustion duration. Further, the rich limit combustion duration is lower than the lean limit duration by about 15 deg CA. This is attributed to the flame speed at the identified lean operation limit being significantly lower than the corresponding rich operation limit (laminar flame speed is 53 cm/s and 42 cm/s at the rich and lean limits of 50 kWe load). Considering the differences in the combustion phasing, the Wiebe coefficients for the rich and lean limit operating condition are estimated and tabulated in table 1. The depicted deviation is from the load average shape factor.

Load	Phi	m	Deviation (%)
40	0.89	2.01	09.5
kWe	1.47	1.83	02.0
50	0.92	2.00	09.9
kWe	1.39	1.85	01.6
60	0.97	1.99	09.3
kWe	1.30	1.91	04.9
70	1.06	2.10	15.1
kWe	1.18	2.06	13.2

Table 1. Shape factor for extreme mixture quality

While the Wiebe coefficients are mixture quality and energy density dependent, the load independent nature of the Wiebe coefficient is brought out in figure 8 where the heat release pattern from no load to 72.8 kWe in steps of approximately 10 kWe closely band together.



Figure 8. Heat release pattern across the complete load range

The minor deviations for 60 and 70 kWe are positioned beyond 80% heat release (CA > 20 deg aTDC) and as such do not affect either the position or magnitude of peak pressure [7].

On the impact of the variation of combustion phasing on 0D

simulations, while the operating point specific shape factors deliver near perfect results, a sensitivity analysis is carried out using two different shape factors. One shape factor is the load average shape factor (S-1) of 1.82 and while the other shape factor is a load dependent linear function for the average of lean-rich shape factors at each of the loads. The idea is to explore the possibilities of using a single number or a function with minimal dependencies for simulating a broad range of operating conditions. The results of the sensitivity analysis are tabulated in table 2 for three loads and the pressure crank angle simulated traces for 70 kWe are presented in figure 9.

	50	60	70
	kWe	kWe	kWe
PoPP-S1	13.0	13.0	13.0
PoPP-S2	12.0	13.0	15.0
PoPP-E(R)	13.0	12.0	12.0
Deviation[E(R):S1]	0.0	1.0	1.0
Deviation[E(R):S2]	1.0	1.0	3.0
PoPP-E(L)	11.0	11.0	12.0
Deviation[E(L):S1]	2.0	2.0	1.0
Deviation[E(L):S2]	1.0	2.0	3.0
PMax-S1	54.3	68.9	74.3
PMax-S2	54.4	68.1	72.7
PMax-E(R)	53.5	67.8	78.8
% Deviation[E(R):S1]	1.5	1.6	5.7
% Deviation[E(R):S2]	1.7	0.4	7.7
PMax-E(L)	60.0	69.3	77.6
% Deviation[E(L):S1]	9.5	0.6	4.3
% Deviation[E(L):S2]	9.3	1.7	6.3

Table 2. 0D simulation sensitivity analysis



Figure 9. Comparison of simulation and experimental traces

It can be observed from the tabulated data that, the maximum deviation experienced between the simulation and experimental results on the position of peak pressure is 3 deg crank angle observed for 70 kWe load with the curve fit shape factor. This is however well within the cyclic average related range. Similar observation can be made with respect to the magnitude of the peak pressure also. Further, across all the loads, simulations using the single load average shape factor of 1.82 are much superior as compared to the curve fit correlations. This could be attributed to the rather sharp divergence in the supported mixture quality and hence the combustion phasing with reducing load. The above results in general permit us to state that a single shape factor can be conveniently used for the simulation of PG fuelled operation of the engine across all the loads and permissible air-fuel range ratio with the deviations being well within the limits of observed cyclic variations.

### 4 Conclusions

The effect of changes in the mixture quality on the combustion phasing has been reported by means of in-cylinder investigations on a natural gas engine fuelled with PG. The mixture quality operating regime for normal operation is seen to be on the richer side which is logical considering that the flame speed for PG peaks on the rich side of stoichiometry. The supported mixture quality range is seen to narrow down on moving towards the higher loads with the rich limit indicating higher sensitivity to load as compared to lean limit and it attributed to the dominance of temperature and mixture quality in reducing the auto-ignition time. While the combustion phasing for PG in general differs significantly from gasoline, across the entire load range, for normal operation with PG, very small deviation, mainly restricted to the top loads is observed. With the variation in mixture quality, along expected lines, significant deviations in the phasing are observed. The Wiebe coefficients for the different heat release patterns are determined based on least square curve fit and the magnitudes indicate a trend in line with the mixture quality regime.

Simulation using a single load average and a load dependent curve fit correlation based shape factors have been carried out. While the single shape factor based simulations remain superior as compared to the curve fit based simulations, overall the deviations are within the cyclic variability for PG operation and such it can be concluded that fairly accurate simulations are possible using fuel specific coefficients that can simultaneously address the load and mixture quality variations.

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