

# Knock and its prediction in producer gas fuelled SI engines

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## Abstract:

A first law based zero dimensional spark ignition engine model with knock predicting abilities is developed to assess the knock limited operating conditions of a producer gas fuelled engine. A cumulative distribution Wiebe function is used to predict the mass burn fraction, and hence the engine heat release, as a function of crank angle. Fuel specific coefficients, from an earlier work by the authors, are used for the Wiebe function towards accurate simulation of the engine. Knock prediction feature is introduced by means of chemical kinetics with detailed chemistry in the unburned mixture. Operating conditions, primarily manifold temperature and pressure that lead to knock are identified in experimental investigations on a producer gas fuelled multi-cylinder turbocharged engine. With end gas auto-ignition resulting from complex interaction of thermal, chemical and fluid parameters, at any operating condition, the range of crank angle within which knock could occur is identified. The generated model is able to predict the knock occurrence within the experimentally determined knock band at each tested operating condition. The model is also able to identify knock occurrence on a different engine configuration at a higher compression ratio where occurrence of knock could not be conclusively established by experimental results.

## 1. Introduction:

The use of bio-derived alternative fuels for fuelling internal combustion (IC) engines is becoming imperative to address the economic and environmental challenges arising out of the use of conventional crude based fuels [1]. Gaseous bio-fuels, prominently, Producer gas (PG), generated from the thermo-chemical conversion of biomass, is becoming increasingly significant due to the possibility of clean burning [2] apart from displacing the use of conventional fuels [3]. In the use of PG to fuel IC engines, it has been recognized that the engine response will differ as compared to the response with conventional fueled operation due to the differences in the thermo-physical properties of PG [4]. The thermo-physical properties of PG are compared with and natural gas (NG) [5] and gasoline (GA) [6] in table 1. One of the important conclusions that can be drawn from table 1 is that, on fuelling a conventional engine with PG, power de-rating can be expected due to the lower

calorific value (LCV), lower adiabatic flame temperature (AFT) and the lower than unity product to reactant mole ratio. The reduction in the power output from baseline power ratings on fuelling with PG has been established for naturally aspirated (NA) operation by the current authors [7] and Dasappa et al [8] for turbocharged after-cooled (TA) operation. It can also be observed that the adiabatic flame temperature (ATF) for PG is low, suggesting lower thermal efficiencies [9].

	GA	PG	NG
A/F (kg/kg)	14.7	1.35	17.0
LCV(gas) MJ/kg	44.0	5.00	50.2
LCV(mix) MJ/kg	2.83	2.12	2.76
AFT (K)	2100	1800	2210
$S_L$ (m/s)	0.42	0.50	0.35
P/R mole ratio	1.06	0.91	1.00

Table 1. Properties of GA, PG and NG

With power de-rating observed under PG fuelled operation, turbocharging of NA engines and turbocharger optimization of existing TA engines

becomes imperative towards operating the engines at the rated loads. Further, towards improving the engine thermal efficiency, the possibility of increasing the engine compression ratio (CR) needs to be explored. The higher laminar flame speed for PG suggests such a possibility. Sridhar et al have reported some improvements in the thermal efficiency by increasing the CR [10].

In order to improve the power output, PG fuelled operation requires pressure boosting and increasing the CR. These two factors are basically knock limited [11] and as such a careful assessment is required before proceeding with turbocharging and increasing the CR. Assessment of the operating conditions that lead to knock, are preferably done using knock predicting models rather than direct experiments considering that knock can have a detrimental effect on the engine structure [12][13].

Conventional engine simulation models, from simple zero dimensional (thermodynamic) to multi-dimensional (fluid dynamic), consider the in-cylinder volume to be broadly divided into burned and unburned zones, separated by an infinitesimally thin flame [9]. The progress of combustion in terms of the fuel-air mixture burn rate is established using experimentally tuned cumulative distribution functions like the Wiebe function [14] or mathematical models of turbulent flame propagation [15]. While these models are capable of closely predicting normal operation, knock prediction features in the form of induction time correlations [9][15] or end gas chemical kinetics models [16] need to be incorporated.

The current work reports on the development of a thermodynamic model with end gas chemistry using a detailed chemical kinetics mechanism for knock prediction for a PG fuelled engine. The choice of thermodynamic model over a

multi-dimensional model was based on the consideration of substantial computational time and resource required for the fluid dynamic models [17]. The cumulative distribution based Wiebe function heat release model is used for the engine heat release. It must be pointed out that, the current authors in a previous work have established PG specific Wiebe parameters [18] as used in the current work against conventional parameters [9] considering that the thermo-physical properties for PG differ significantly. Towards validation of the developed model, the predicted knock occurring crank angle (KOCA) is compared with experimental observed knock results for a PG fuelled multi-cylinder engine. The generality of the model is established by comparing the results for a different engine configuration.

## **2. Methodology:**

Experiments were conducted at a fixed speed (1500 rpm) and compression ratio (CR=10.5) on a Cummins India Limited (CIL) make turbocharged and after-cooled, six cylinder engine rated at 90 kWe in diesel mode. The engine has been converted for NG operation and subsequently adopted for PG fuelled operation. A spark plug adapted pressure sensor was mounted by replacing the conventional spark plug on one of the cylinders to acquire the in-cylinder pressure trace as a function of crank angle at steps of 0.1 deg CA. Details of the engine and the instrumentation can be found in [7][18]. The maximum brake torque (MBT) ignition timing was first established based on a spark sweep test and the knock limited peak supported load was determined. At various loads, for a fixed mixture quality, the KOCA was determined as a function of manifold temperature. Knock detection, primarily the KOCA, was based on the spectral

analysis of the pressure crank angle traces.

A zero dimensional model with Wiebe heat release coupled with a chemical kinetics model to predict end gas auto-ignition is developed. The details of the model are presented in the next section.

### 3. Modeling

The model is fundamentally based on the first law of thermodynamics that simulates the evolution of the cylinder pressure (P) as a function of crank angle ( $\theta$ ) given the volume (V) change and heat transfer (Q). The governing equation for the closed system is as given below where,  $\gamma$  is the polytropic index.

$$dP/d\theta = (\gamma-1)/V * \delta Q/\delta\theta + \gamma(P/V)(dV/d\theta)$$

The model at the basic level starts with the four bar kinematics with the rotation of the crank shaft translating into the linear motion of the gudgeon pin axis. With the cylinder volume change as the driving force, the gas exchange sub-model, based on the filling and emptying technique [9] is invoked for the duration when the engine cylinder acts like an open system and the mixture intake and burned gas scavenging is taken care of. The valve lift profiles of the engine are available from the manufacturer, while the coefficient of discharge is modeled as a function of the lift to diameter ratio [19]. With the engine being non adiabatic, heat transfer between the gas and the engine walls ( $Q_w$ ) is estimated from the Newton's law of cooling, with the spatially average convective heat transfer coefficient ( $h_{cg}$ ) being estimated from the Annand's correlation [20]. The coefficients are tuned to match the simulation results with the experimental motoring curves. In the Newton's equation below,  $T_g$  and  $T_w$  represent the gas and wall temperatures respectively.

$$dQ_w/dt = h_{cg}(T_g - T_w)$$

The model at this stage is able to simulate a typical motoring pressure trace. Beyond this stage, as a strategy, two parallel models are developed which are subsequently merged to evolve a 0D knock predicting model. The first model adopts the Wiebe function where heat is considered to be added from across the system boundary. In the Wiebe function given below,  $X_b$  is the mass fraction burned expressed as a function of the instantaneous crank angle  $\theta$ , start of combustion angle  $\theta_{soc}$ , duration of combustion  $\Delta\theta_{doc}$ , shape factor 'm' and efficiency factor 'a'.

$$X_b = 1 - \exp\{-a[(\theta - \theta_{soc})/\Delta\theta_{doc}]^{m+1}\}$$

The shape and efficiency factors are experimentally tuned for PG reported by the authors in a different work [18] and accordingly, the model can accurately predict the pressure trace development for normal combustion [18]. While the above model can accurately predict normal combustion, it cannot predict end gas auto-ignition since the unburned gas ahead of the flame is considered to be chemically frozen and as such lacks the auto ignition mechanism. Towards releasing the frozen chemistry constraint, a homogeneous charge compression ignition (HCCI) model is developed wherein the entire mixture is considered lumped with no heat addition either externally as in the Wiebe function or internally by flame propagation. With the change in crank angle, as the mixture undergoes a thermodynamic state change, chemical kinetics considering 53 species in a reaction mechanism involving 325 reactions is invoked. With the chemical time step of the order of  $1.0 \times 10^{-8}$  s as compared to  $1.1 \times 10^{-4}$  s physical step (corresponding to 1 deg CA), the system is treated as isochoric. As the crank angle

and hence the volume change, the mixture density and concentration get updated. At each crank angle, the change in the specie concentration and hence the enthalpy, pressure and temperature of the mixture is evaluated by simultaneously solving for all the specie concentration change rate equations. The chemical kinetics system with a set of nonlinear ordinary differential equations represents a stiff system and a semi-implicit scheme involving linearizing the system of equations is implemented [21]. If the necessary conditions are attained during the course of the cycle, the entire mixture auto-ignites, leading to instantaneous release of energy and accordingly rise in the temperature and pressure.

Towards realizing the knock model, the HCCI model is merged with the Wiebe function based model wherein, the unburned gas experiences temperature and pressure rise due to engine kinematics as well as the heat release due to burning of the mixture. If the end gas ignition delay time is less than the time for the complete consumption of the end gas mixture then the remaining mixture, represented by the unburned mass fraction auto-ignites, representing knock, and leading to a spike in the pressure and temperature. The crank angle at which such a spike in the pressure is observed is established as the KOCA. The results are discussed in the next section.

## 4. Results and discussions

### 4.1 Experimental results

The spark sweep test yields the MBT ignition timing at 22 deg before top dead center (TDC), advanced by 6 deg as compared to the NG MBT ignition timing of 28 deg before TDC. The ignition advance is attributed to the higher flame speed for PG over NG. Towards establishing the peak supported load at MBT, the engine is gradually raised to a

load where small abnormalities on the pressure trace, indicative of incipient knock start to appear. The engine supports a peak load of 72.8 kWe beyond which end gas auto-ignition is evident on the pressure traces. Figure 1 presents the 250 cycle ensemble average pressure crank angle traces at the top three loads (restricted for brevity). The outcome of the spark sweep test is indicated as inset data.

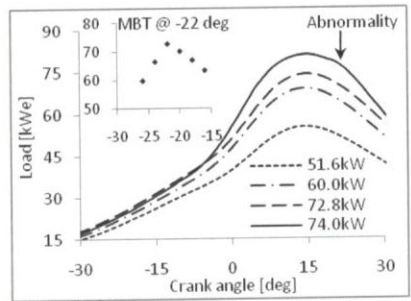
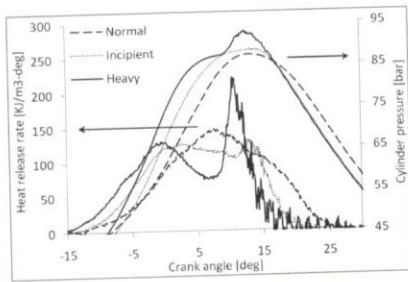


Figure 1. MBT P-0 traces and spark sweep test

It is to be noted that, while the turbocharger is able to support mixture flow rates for even higher loads (the engine was loaded momentarily to 78 kWe to capture heavy knock), the limitation is on the after-cooler. A simple analysis indicates that the air flow rate handled by the after-cooler for diesel operation is about 356 kg/h at 90 kWe (SFC of 0.22 kg/kWh and A/F ~ 18) while for PG at 72.8 kWe the flow rate is already 427 kg/h. With an increase in the flow rate through the after-cooler, it is unable to maintain the required inlet manifold temperature leading to end gas auto-ignition. Hence the peak load achieved is knock limited.

Knock detection based on the acquired in-cylinder pressure is possibly the most accurate of the available methods [22] considering that the auto-ignition triggered acoustic signals are directly picked up by the pressure sensor. While the simplest way to detect knock would to

check the pressure signal for discrepancies, the heat release rate curve, derived from the pressure trace [9] also gives a very good indication.

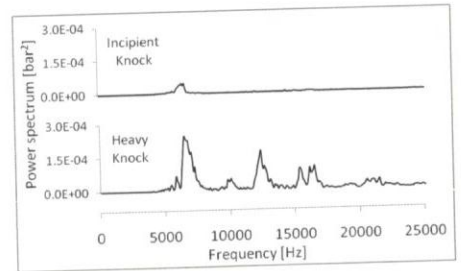


**Figure 2. P- $\theta$  and heat release curves for normal and knocking combustion**

Figure 2 shows three P- $\theta$  and differential heat release rate traces corresponding to normal, incipient knock and heavy knock. It can be observed that, the near symmetric profile of normal combustion gets distorted with incipient knock while the high frequency fluctuations are evident for heavy knock. The discrepancies in the pressure profile are more clearly evident on the derived heat release trace. The uni-modal nature of the heat release trace for normal combustion, which signifies a progressive and controlled heat release, gets distorted to bio-modal nature as there is a sudden release of energy due to the end gas auto-ignition. The bi-modal nature of the heat release trace is also a clear indicator of knock. It can also be observed that the second spike due to the sudden energy release, especially for heavy knock, is substantially higher with higher rate of rise than the flame propagation related heat release. This is primarily due to the fact that end gas auto-ignition is almost akin to constant volume heat release.

While visual observation gives a good indication of knocking cycles, with 750 cycles per minute, its utility is restricted to offline processing and also the estimation of the KOCA is imprecise.

Towards online estimation of knock and KOCA, the pressure signal is subjected to spectral analysis (Fast Fourier transformation) since, it has been established that, knock excites characteristics frequencies in the 5 kHz to 7 kHz range [9] and a presence of these frequencies in the spectrum indicates knock.



**Figure 3. Spectral analysis of cylinder pressure signal at 74 kW**

Figure 3 presents the results of spectral analysis of incipient and heavy knocking cylinder pressure signal. It can be observed that, in both the cases, the first peak is shown in the vicinity of 7 kHz which is the natural vibration of the first order transverse mode of the gas and is a clear indication of knock [23][24]. With the identification of knocking cycles, the next task is to identify the KOCA. Towards this, the cylinder pressure is passed through a low pass filter with a 4000 Hz cutoff frequency and the filtered pressure signal is subtracted from the raw signal. This leaves only the high frequency components and plotting the same as a function of crank angle gives the KOCA. The first appearance of the high frequency components can reasonably be considered as the KOCA. It is important to note that, auto-ignition itself will have occurred slightly earlier and there is some lag by the time the signal reaches the sensor. Figure 4 presents the filtered pressure traces for the normal combustion and incipient and heavy knocking. The KOCA has been

indicated for the incipient and heavy knock cycles.

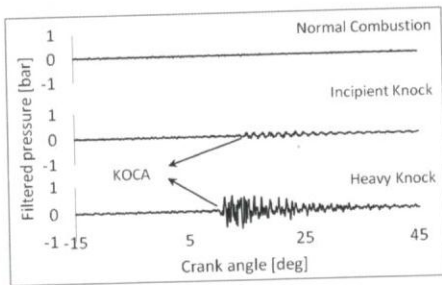


Figure 4. Filtered pressure signal to detect high frequency components and KOCA

Having established the method for identifying knocking cycles and the KOCA, experiments are extended to identify the manifold temperature and pressure at various loads for which engine knocks. At each of the loads, the after-cooler water flow rate was controlled till such time that the spectral analysis indicated knock. Table 2 below consolidates the manifold temperature and pressure corresponding to knocking operation at the considered loads.

Load (kWe)	Pressure (bar)	Temp (K)
72.8	1.86	314.15 ± 1
70.0	1.80	315.15 ± 1
60.0	1.71	321.15 ± 1
50.0	1.47	328.15 ± 1

Table 2. Knock limiting temperature and pressure at various loads

It is evident that, with increasing load, the knock limiting manifold temperature reduces. This is along expected lines considering that with increase in the load while the energy input to the cycle increases, making the engine to run hot, the rise in the manifold pressure (due to boosting) causes an overall increase in the mixture temperature as it is compressed. It is also important to note that, at any

given temperature and pressure when knock is observed on the pressure trace, cycle by cycle there is no repeatability of knock both in terms of KOCA and the magnitude. Accordingly, at each operating condition, a KOCA band rather than a single KOCA is identified.

In the discussion on properties of PG, it was brought out that engine operation at higher CR is one of the possibilities. In a work on PG, Sridhar et al [10] report on PG fuelled engine operation at a high CR of 17. The engine was a single cylinder 28 kWe (RB33) Kirloskar make diesel engine converted for PG operation. Figure 5 presents the pressure and pressure rise rate profile development with crank angle at CR17. While the pressure crank angle trace does not indicate any knock like characteristics, possibly due to the limitation on the instrumentation resolution, the pressure rise rate is seen to exceed 10 bar/deg while the general recommended limit is less than 5 bar/deg [25].

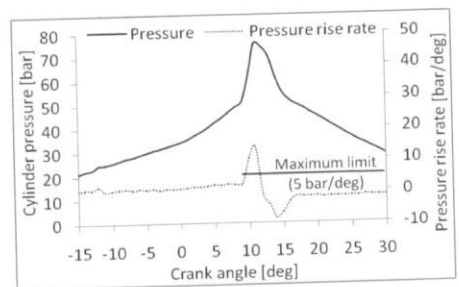


Figure 5. Pressure and pressure rise rate at CR of 17 for a different engine configuration [10].

The above case exemplifies a situation wherein knock detection based on the experimental traces is not straight forward and knock predicting model is to be used.

#### 4.2 Modeling and simulation results

At different stages of model development, various sub-modules have been validated with literature published results. Some of the critical validation

results are discussed before presenting the actual simulation results.

On the simulation of the engine cycle for normal combustion, the Wiebe function based heat release is a critical module since the pressure development is only as accurate as the heat release pattern. The Wiebe function relies on the shape and efficiency factors towards generating the mass burn profile as a function of crank angle. Literature suggests a value of 2 for the shape factor and 5 for the efficiency factor [9] for the conventional fuels. Using these parameters resulted in near complete failure of simulation as indicated in figure 6 below.

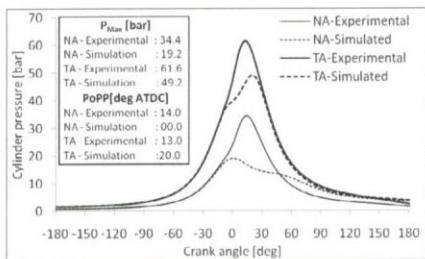


Figure 6. Experimental and simulation (conventional coefficients) results comparison.

The substantial deviation of simulation results from experimental results on using conventional Wiebe coefficients is attributed to the difference in the heat release profile development for PG fuelled operation. This required PG specific coefficients of 2.4 and 0.7 for the efficiency and shape factors respectively. The authors, in a different work [18] have addressed the details of the difference in the heat release pattern and the selection of the PG specific Wiebe coefficients.

Figure 7 compares the simulation results using PG specific Wiebe coefficients with the experimental results at two different loads. As is evident, a near perfect match is obtained on the overall profile in general and the position of peak pressure in particular. This

validates the model for normal engine operation.

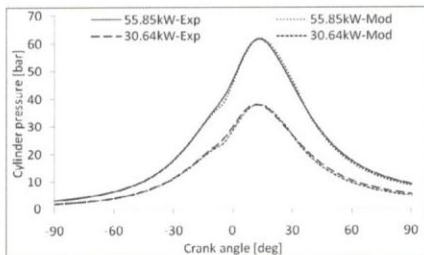


Figure 7. Experimental and simulation (PG specific coefficients) results comparison.

Having validated the engine model for normal combustion, the chemical kinetics model for end gas auto-ignition is validated. Towards validation of the chemical kinetics model, the specie evolution and auto-ignition time for CH<sub>4</sub> – air mixture in a constant volume bomb under isobaric and adiabatic conditions is compared with the results from CHEMKIN [26], the industry standard for simulation of complex chemical reactions. Figure 8 compares the evolution of major species with the continuous lines indicating the results from the code and symbols indicating the results from CHEMKIN. It is evident that the developed chemical kinetics module is evolving the species accurately.

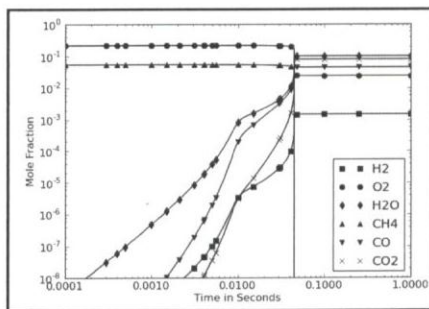


Figure 8. Specie profile evolution for stoichiometric methane-air auto-ignition.

Towards further verification, the specie evolution and auto-ignition time

for propane air mixture and H<sub>2</sub>-air mixture is compared with CHEMKIN results and literature reported simulation and experimental results [27].

Having validated the chemical kinetics module, a HCCI model is generated by integrating chemical kinetics sub-module with the engine module but without the Wiebe function so that ignition is purely controlled by chemical kinetics. Towards verifying the HCCI model, literature reported simulation results were considered [28] and using similar kinematics and initial conditions, simulations were carried out. Figure 9 shows the simulation result for H<sub>2</sub>-air HCCI engine. The continuous lines indicate the current simulation results while the dots indicate the literature reported value (shown at only one temperature from brevity).

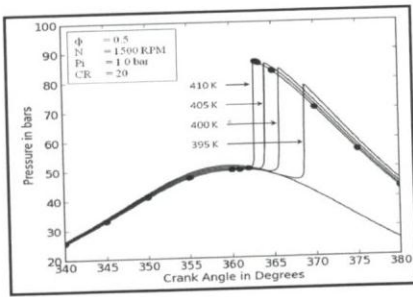


Figure 9. H<sub>2</sub>-air fuelled HCCI simulation

Having validated the various sub-models, simulations using the full chemistry engine simulation model are carried out to assess its ability to predict knock.

Figure 10 presents the knock simulation results for the three loads of 50, 60 and 70 kWe. The inlet pressure and temperature for the simulation at these three loads is mentioned in table 2. The experimental knock band excluding the outliers is indicated inset. It is important to note that, the parameters that induce cycle to cycle variations in an engine [9] also have an impact on the

engine knock both on the intensity and the KOCA. The analysis of the knocking cycles clearly indicates the existence of a range. Hence, while the simulation results indicate a single KOCA, in practice, it is a band within which knock occurs.

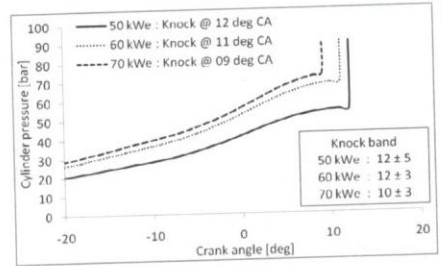


Figure 10. Knock simulation results

It can be observed from figure 10 that, at each of the operating conditions, the model predicts the knock within the corresponding band. Further, with increasing load, the KOCA is seen to shift towards the TDC. This is logical considering that the prevailing conditions in the cylinder would be much severe at higher loads and as such knock occurs much earlier in the cycle.

Having established the ability of the developed model as a tool for predicting knock, the generality of the model is put to test by trying to analyze the pressure evolution for the operating conditions for RB33. The normal combustion pressure trace is simulated by the model near perfectly at two different CR's of 11.5 and 13.5 respectively [18]. Of particular interest however was the experimental result obtained at CR 17 as presented in figure 5. On initializing the model with conditions pertaining to CR17 [10], simulations yield an interesting result presented in figure 11 wherein, auto-ignition is shown to occur in the vicinity where experimental results have indicated a sharp rise in pressure. While no knock like characteristics are evident on the experimental pressure trace, simulation results clearly point to end gas auto-



ignition. The model has been successful in identifying end gas auto-ignition even when the same is not explicitly evident.

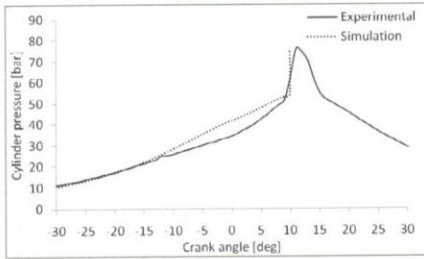


Figure 11. Knock simulation for high CR engine with different in-cylinder geometry

## 5. Conclusion and Outlook

A zero dimensional Wiebe function based model with PG specific coefficients and end gas chemistry has been developed towards predicting knock limited operation of the engine. Knock, captured on a multi-cylinder engine and identified by the spectral analysis of the pressure signal reveals a band of crank angle rather than a single value within which the knock gets initiated. The developed model is able to predict knock occurrence within the band of crank angle for each of the tested operating condition. The model is able to predict knock even on a different engine geometry wherein knock was not explicitly evident. The developed model can be used for establishing the knock limited operation condition for any fuel by adopting appropriate Wiebe coefficients.

## 6. Acknowledgement

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