

## Experimental and Skeletal Kinetic Model Study of Compressed Natural Gas Fueled Homogeneous Charge Compression Ignition Engine

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**Abstract: Problem statement:** In homogeneous charge compression ignition engines fuel oxidation chemistry determines the auto-ignition timing, heat release, reaction intermediates and the ultimate products of combustion. To shorten development time and to understand combustion processes, the use of simulation is increasing. **Approach:** A model that correctly simulates fuel oxidation at these conditions would be a useful design tool. Detailed models of hydrocarbon fuel oxidation, consisting of hundreds of chemical species and thousands of reactions. A way to lessen the burden was to use a skeletal reaction model, containing only tens of species and reactions. **Results:** The model was developed from the existing pre-ignition model, which had 10 species, 5 elementary reactions for kinetic and 6 elementary reactions for equilibrium and the standard k- $\epsilon$  turbulence model had been used in this investigation. This model combines the chemistry of the low, intermediate and high temperature regions. **Conclusion:** Simulations are compared with measured and calculated data from the engine operating at the following conditions: speed 1500 RPM, inlet temperature 363-433 K, fuel CNG and  $\lambda$  range 3-5. The simulations are generally in good agreement with the experimental data including temperature, pressure, combustion duration and ignition delay and heat release.

**Key words:** Internal combustion engine, top dead centre, spark ignition, compression ignition

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### INTRODUCTION

Internal combustion engines have been widely used in numerous applications throughout the world. A new mode of combustion is being sought in order to reduce the emission levels from vehicles and one of the new modes is Homogeneous Charge Compression Ignition (HCCI) engines. HCCI is defined as the process by which a homogeneous mixture of air and fuel is compressed under conditions that auto-ignition occurs near the end of the compression stroke, followed by the combustion process that is significantly faster than conventional diesel or Otto combustion (Rattanapaibule and Aung, 2005). It can provide high efficiency while maintaining low emissions and can be used in both modified Spark Ignition (SI) and Compression Ignition (CI) engines with any fuel or combination of fuels. The mixture in HCCI engines auto-ignites in multiple spots and is then burned volumetrically without discernable flame propagation (Kong and Reitz, 2002). Combustion takes place when the homogeneous fuel mixture has reached the chemical activation energy and is fully

controlled by chemical kinetics rather than spark or injection timing.

Since the mixture is lean and fully controlled by chemical kinetics, there is a new challenge in developing HCCI engines as it is difficult to control the auto-ignition of the mixture and the heat release rate at high load operation, achieve cold start, meet emission standards and control knock (Kong and Reitz, 2003; Soylu, 2005).

The advantages of HCCI engine are:

- The same or even better power band compared to SI or CI engines
- High efficiency engines due to no throttling losses and high compression ratio
- Ability to be used in any engine configuration: automobile engines, stationary engines, high load engines or small size engines

However, HCCI engines have their own disadvantages such as high level of Unburned

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Hydrocarbons (UHC) and CO (Kong and Reitz, 2003; Nathan *et al.*, 2010; Yap *et al.*, 2006) as well as knocking issues if the mixture is relatively inaccurate (Kong and Reitz, 2003; Nathan *et al.*, 2010; Jun *et al.*, 2003). Emissions regulations are becoming more stringent and even though CO, NO<sub>x</sub> and smoke emissions level in a HCCI engine have been reduced while maintaining efficiencies close to those of diesel CI engines (Soylu, 2005), knocking is still the major issue because of its sudden onset. Knocking is due to premature combustion where the ignition takes place before the piston reaches Top Dead Centre (TDC) and it reduces engine reliability due to high vibration effects.

It is well known that the fossil fuel reserves all over the world are diminishing at an alarming rate and a shortage of crude oil is expected at the early decades of this century (Aslam *et al.*, 2006). Probably in this century, it is believed that the crude oil and petroleum products will become very scarce and costly to find and produce.

Gasoline and diesel fuel will become scarce and most costly (Catania *et al.*, 2004). Alternative fuel technology, availability and use will become more common in the coming decades for internal combustion engines. Nowadays, the alternative fuel has been growing due to concerns that the reserves of fossil fuel all over the world are finite and at the early decades of this century will run out completely. Furthermore, the current world energy crisis makes the fossil fuel price increase. On the other hand, the fossil fuel contributes large environment pollution. Many types of alternatives fuels are available in this world. Compressed Natural Gas (CNG) as an alternative fuel is becoming increasingly important.

The detailed models can be culled to produce a second type of model, the reduced model. These models contain the most critical elements of the full mechanism. A third form of model is the skeletal model that consists of a sequence of composite kinetic steps representing the reaction progress. These kinetic steps can be elementary, generic, or global reactions. Rate parameters and thermo chemistry are based on the best information but represent classes of reactions. Using skeletal models, pre-ignition behaviors, ignition time and combustion rate of HCCI engine have been predicted (Zheng *et al.*, 2001; 2002). The results show the skeletal model can be a useful tool to study HCCI engine operation.

In CNG fueled HCCI engines, compression due to piston motion and heat release resulting from preignition chemical reactions produce in-cylinder pressures and temperatures which eventually lead to ignition and combustion. During this heat release process, chemistries characteristic of the low,

intermediate and high temperature regions play a critical role (Nathan *et al.*, 2010). In order to understand these processes, chemical models must be developed.

**Structure of the skeletal chemical kinetic model:** In engineering, modeling a process means to develop and use the appropriate combination of assumptions and equations that permit critical features of the process to be analyzed. Engine models describe the thermodynamic, fluid flow, heat transfer, combustion and pollutant formation phenomena in engines. Examples of labels given to engine models are zero-dimensional, quasi dimensional and multi-dimensional models. These can also be categorized as thermodynamic or fluid dynamic in nature, depending on whether the equations which give the model its predominant structure are based on energy conservation or on a full analysis of fluid motion. In Multi-Dimensional models, the full governing differential conservation equations of physics with time and spatial dimensions are solved for the processes in the engine. Many sub-models, such as turbulence and combustion models, are still needed to avoid the need for direct calculation of the Navier-Stokes equations and chemical reactions. Detailed boundary and initial conditions are also necessary. Numerical methodologies are introduced to approximate the differential equations by their algebraic counterparts whose dependent variables are the values of the velocities, pressure, temperature, at the nodal points of a computational mesh. Obviously knowing at what conditions of temperatures, pressures and compositions a methane-air mixture can ignite, is very important in optimization of an engine performance in CNG fueled HCCI engine. A fundamental understanding of the thermodynamics and fuel composition related factors influencing combustion in internal combustion engines can only be obtained from a detailed study of the processes.

**Governing equations:** This simulation divides the complete cycle into the overlap, intake, compression, combustion, expansion and exhaust processes. In each of these processes the governing equations of fluid flow and chemical reactions are solved in a skeletal reaction model.

Continuity Eq. 1:

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \vec{u}) = \nabla \cdot \left[ \rho D \nabla \left( \frac{\rho_m}{\rho} \right) \right] + \rho_m^c + \rho_m^s \delta_{ml} \quad (1)$$

Momentum Eq. 2:

$$\frac{\partial}{\partial T}(\rho\bar{u}) + \nabla \cdot (\rho\bar{u}\bar{u}) = -\frac{1}{a^2}\nabla p - A_o\nabla\left(\frac{2}{3}\right)\rho k + \nabla\sigma + \bar{F}^s + \rho g \quad (2)$$

Turbulence kinetic Eq. 3:

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho\bar{u}k) = -\frac{2}{3}\rho k\nabla\bar{u} + \sigma\nabla\bar{u} \cdot \left[ \left( \frac{\mu}{\rho r_k} \right) \nabla k \right] - \rho\varepsilon + W^{*s} \quad (3)$$

Epsilon Eq. 4-7:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho\bar{u}\varepsilon) = -\left[ \frac{2}{3}C_{\varepsilon 1} - C_{\varepsilon 3} + \frac{2}{3}C_{\mu}C_{\eta}\frac{k}{\varepsilon}\nabla \cdot \bar{u} \right] \rho\varepsilon\nabla \cdot \bar{u} \quad (4)$$

$$-\frac{\varepsilon}{k}\left[ (C_{\varepsilon 1} - C_{\eta})\sigma : \nabla\bar{u} - C_{\varepsilon 2}\rho\varepsilon + C_s W^{*s} \right] + \nabla \cdot \left[ \left( \frac{\mu}{Pr_k} \right) \nabla\varepsilon \right]$$

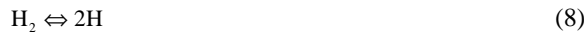
Where:

$$C_{\varepsilon 1} = 1.42, C_{\varepsilon 2} = 1.68, C_{\varepsilon 3} = 0.41333 + (-1)^s 0.06899C_{\eta}\eta \quad (5)$$

$$C_{\eta} = \frac{\eta(1 - \eta/\eta_o)}{1 + \beta\eta^3}, \begin{cases} \delta = 1 & \text{if } \nabla \cdot \bar{u} \leq 0 \\ \delta = 0 & \text{if } \nabla \cdot \bar{u} \geq 0 \end{cases} \quad (6)$$

$$\eta = S\frac{k}{3}, S(2S_{ij}S_{ij})^{\frac{1}{2}}S_{ij} = \frac{1}{2}\left( \frac{\partial\mu_i}{\partial x_i} + \frac{\partial\mu_j}{\partial x_j} \right) \quad (7)$$

**Chemical equations:** The following species has been used for compressed natural gas (CNG) combustion; Fuel, NO, O, N<sub>2</sub>, O<sub>2</sub>, N, H<sub>2</sub>, OH, CO, CO<sub>2</sub> and the following equations have been considered for chemical equilibrium in combustion calculations Eq. 8-13:



**Chemical kinetics:** The model assumed single step oxidation of Compressed Natural Gas (CNG) with oxygen to form carbon dioxide and water vapor Eq. 14:



The reaction rate for this single step has been used is the global one-step methane oxidation reaction rate proposed by Westbrook and Dryer (1981) in standard SI units Eq. 15:

$$\frac{dCH_4}{dt} = -130 \times 10^6 \exp\left(\frac{-24400}{T}\right) [CH_4]^{-0.3} [O_2]^{1.3} \quad (15)$$

The extended Zeldovich kinetic equations have been used for calculation of NO emission Eq. 16-18:



**Experimental apparatus and procedure:** The data used in this study are from a single cylinder, four stroke, air cooled research engine. In its present configuration, the engine has a 114.3 mm bore, a 139.7 mm stroke and a 17.5 compression ratio. A key feature of the facility is the ability to preheat the intake charge over a range of temperature, 300-500 K and to independently control the manifold pressure. The engine operates at a constant engine speed of 1500 rpm. Fresh air fuel mixture is mixed in the gas carburetor and inducted into the combustion chamber. A Kistler 6125 pressure transducer located at the rear of the combustion chamber along the axis of the pent-roof was amplified with a Kistler 504E charge amplifier. Crankshaft position was measured with a Dynapar crankshaft encoder and a hall-effect sensor provided camshaft location. Cylinder pressure data was recorded using the MTS-DSP Advanced Combustion Analysis Program (ACAP) that calculates performance parameters such as Peak Pressure and location of peak pressure in real time.

The experiments were conducted with constant fueling, as a result, changing intake air temperature which led to small changes in the mass based  $\lambda$ . This is due to the volumetric nature of air induction into the naturally aspirated engine and as a consequence,  $\lambda$  values are not constant but rather presented as a narrow range. A single engine speed of 1500 RPM was used.



Fig. 1: Experimental setup

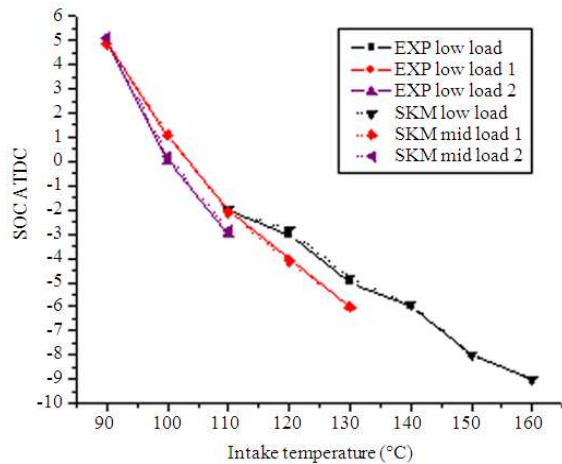


Fig. 2: Experimental and simulation of start of combustion versus Intake temperature at three load condition

Table 1: Thermal management test conditions

	Engine load		
	Low	Mid-1	Mid-2
$\lambda$ range	5.0-4.2	4.0-3.5	3.2-3.0
Fueling rate (g/sec)	1.43	1.84	2.24
Fuel input energy rate (kW)	42.5	54.6	66.5
Intake temperature range (°C)	110-160	90-130	90-110
Load range (Nm)	48-55	59-93	118-128
IMEP range (kPa)	221-236	233-318	383-403

This speed corresponded to the manufacturers specified engine speed at rated torque; it was selected to ensure smooth, well balanced engine operation free of resonant vibrations. Table 1 summarizes the three load conditions explored, the intake temperature ranges used and the performance characteristics of each range.

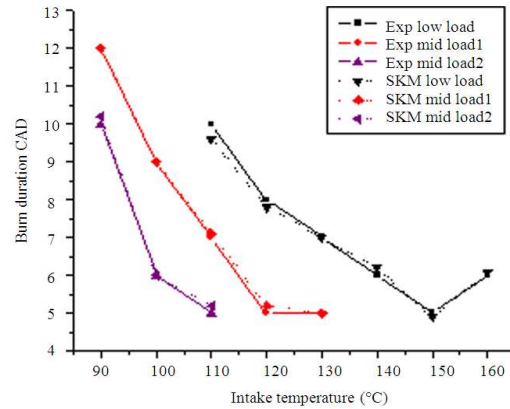


Fig. 3: Experimental and simulation study of burn duration versus Intake temperature at three load condition

Using measured pressure data, the core temperature and heat release was calculated using a locally modified version of a standard Heat Release Model (HRM) (Ferguson *et al.*, 1987). The Skeletal Kinetic Models (SKM) was modified to simulate the core temperature using the same methodology as the heat release model (Zheng *et al.*, 2002) and then was tested using the rate parameters suggested by Li *et al.* (1996) for CNG fuel specific rate parameters adjusted in order to adapt the model to the specific test fuels. Using these rate parameters, the temperature and heat release were simulated and compared with experimental data for different inlet temperatures, equivalence ratios and engine loads (Fig. 1).

The combustion durations were calculated for a number of inlet temperatures using the skeletal model for CNG fueled HCCI engine combustion. Results of simulations and experiments are shown in Fig. 3. Combustion duration is calculated as the CAD difference between 10 and 90% mass fraction burned. In general, combustion duration calculations agree well with experimental data. The dotted line represent skeletal kinetic model results and continuous line represent experimental results as shown in Fig. 3. It can be clearly seen that at all engine loads studied elevating intake temperatures leads to advances in SOC as shown in Fig. 2. More advanced combustion in turn leads to higher peak heat release rates. With more heat released prior to or very near TDC, the physical volume in which the energy is released becomes smaller and due to engine geometry, does not change as much per CAD. This causes higher cylinder pressures and consequentially higher temperatures. Advanced SOC leads to higher heat release rates and higher in-cylinder temperatures leading to elevated cylinder liner temperatures which increase the vapor pressures and evaporation rates of organic compounds in the lubricating oil.

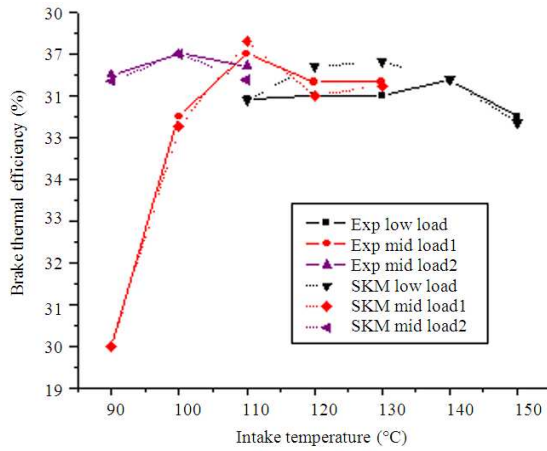


Fig. 4: Experimental and simulation study of brake thermal efficiency versus Intake temperature at three load condition

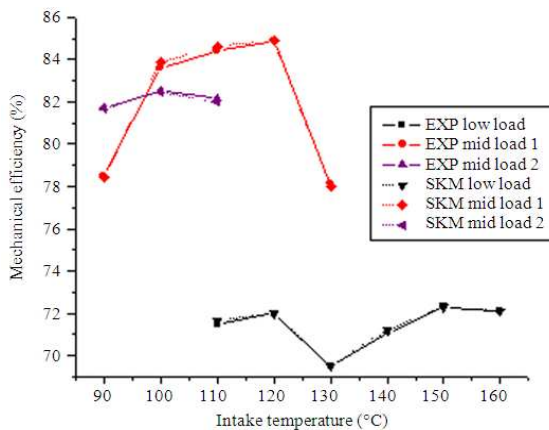


Fig. 5: Experimental and simulation study of mechanical efficiency versus Intake temperature at three load condition

Brake and Indicated thermal efficiencies are generally used to express the efficiency of an engine. Figure 4 and 5 shows the efficiencies obtained from both model predictions and measurements. As the engine intake temperatures are increased, the most notable jumps in combustion efficiency are seen near the lowest intake temperatures. At these temperatures the fuel conversion begins to deteriorate as in-cylinder temperatures, in the coolest regions of the combustion chamber fall below those required for full oxidation of the fuel. Figure 6 depict the comparison of the model predictions and measurements for peak temperature over the entire operating range. Similarly, Fig. 7 depicts the comparison of the model predictions and measurements for peak HRR over the entire operating range.

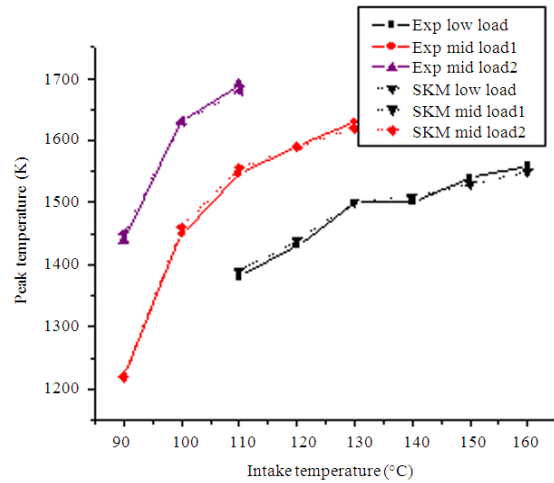


Fig. 6: Experimental and simulation study of Peak Temperature versus Intake temperature at three load condition

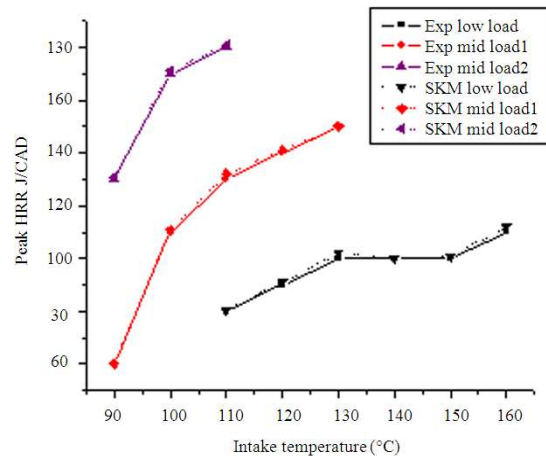


Fig. 7: Experimental and simulation study of peak HRR versus Intake temperature at three load condition

The HRR is an important parameter to identify the onset of knock. At other operating conditions, the model matched the experimentally observed ignition time quite well and the model satisfactorily reproduced the experimental pressure and temperature histories. However, near the HCCI operating boundaries deviations in the HRR began to appear, consistent with the extreme sensitivity of HRR calculations to small variations in measured pressure data. In both the simulations and the experimental data, the first stage ignition occurs at temperatures around 725 K and the second stage ignition occurs at temperatures around 1000 K. Higher intake temperatures lead to higher in-cylinder temperatures through advanced combustion.

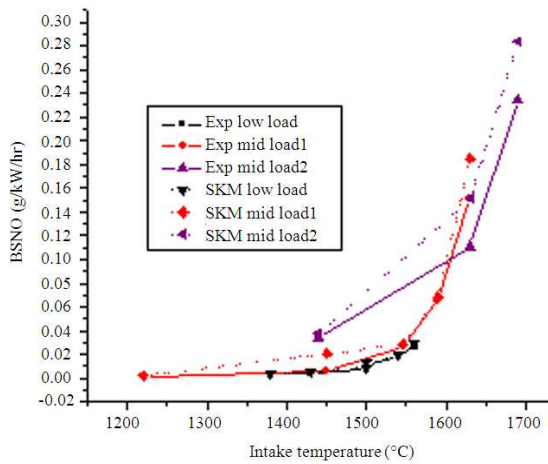


Fig. 8: Experimental and simulation study of BSNO<sub>x</sub> versus Intake temperature at three load condition

These thermal conditions, promoting more complete oxidation of hydrocarbons, also lead to increasing NO<sub>x</sub> levels. HCCI operation is generally characterized as a low NO<sub>x</sub> technique; the knocking behavior when running with pure CNG raised the peak combustion temperature to a value well above normal combustion and the critical Zeldovich NO<sub>x</sub> production threshold, giving very high NO<sub>x</sub> emissions. Figure 8 depicts the comparison of the model predictions and measurements for BSNO<sub>x</sub> emissions over the entire operating range. Both gas phase and particulate brake specific emissions exhibit very clear dependencies on intake air temperature.

Uncertainty exists in both computational and experimental results. The uncertainty can exist in the form of bias and precision errors. With careful calibration, the bias error can be minimized. The precision error can possibly be reduced through assuring that the engine is at steady state operating conditions and the sample interval and frequency are adjusted to properly resolve the process. The discussion of the bias errors will focus on the fuel and the in-cylinder pressure measurements, since they are important for determining the combustion characteristics and cycle thermal efficiency. Within the range of typical HCCI fuel measurements, which for this study were on the order of 0.16 g sec<sup>-1</sup>, the accuracy of a state of the art fuel meter, at these low fuel flow rates, is on the order of 2%. Other methods can be used to check the fuel measurement, but these methods also exhibit errors that can propagate through the calculations. The pressure transducer has linearity within 0.1%, so the transducer itself can be assumed to be very accurate. Since the dynamic piezo-electric pressure transducer can measure only relative changes

in pressure, the absolute pressure level has to be referenced. The encoder alignment can also be off anywhere from 0-1 ca-degrees depending on the alignment procedure. There are several methods, both mechanical and thermodynamic, can be used to either align the encoder or find its offset from true engine TDC.

## CONCLUSION

A skeletal kinetic model describing the chemistry of the CNG fueled HCCI combustion process in engines has been developed. Key features of the model include provision for atom conservation and linking of both a high temperature sub-mechanism and a large molecule decomposition model with a low and intermediate temperature pre-ignition model. The model has been validated against experimental data and the following observations and predictions can be made about the skeletal kinetic model. The skeletal model can simulate the NTC behavior based on the degenerate branching mechanism. The first stage ignition temperature is around 725 K. The second stage ignition temperature is around 1000 K. The skeletal model has successfully predicted HCCI engine behavior including ignition time, rapid combustion duration and heat release. As expected, model predictions confirm that the ignition time is sensitive to the inlet temperature and that this further affects the indicated efficiency of the engine greatly. Other factors affecting ignition timing still need to be examined. The present skeletal model can be a useful tool to study HCCI engine operation. Future work will involve enhancing the model to handle mixtures of fuels, including alkenes and aromatics in order to evaluate the effects of fuels on the HCCI combustion. The ultimate goal is to simulate HCCI behavior including CO and HC emissions for real world fuels.

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