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The Numerical Modeling of Internal Combustion Engines with Application to Simulation of Combustion of Single-Cylinder HCCI engine by Cantera and Application of Implementation of an Integrative MATLAB Engine Model and Validation on Waukesha VHP Series Engines

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ABSTRACT

Internal Combustion Engines will continue to be one of the main sources of power with a demand to control the produced emissions and increase efficiency. The Mathematical modeling of Engines is done by different software and in this paper we will demonstrate two software's that could serve the target mentioned. Cantera & MATLAB namely

The First model will be through Cantera Modeling of the combustion behavior of a homogeneous charge compression ignition (HCCI) engine is unpredictable due to the fact that the technology is recent. Chemical kinetics entirely governs combustion, and varying input parameters have an effect on the mixture's chemical reaction. Reference (9,10 & 11)

The Second Model will be the Integrative MATLAB Engine Model and Validation on Waukesha VHP Series Engines References(1 to 5)

Introduction

In a homogeneous-charge compression-ignition (HCCI) engine, a nominally homogeneous fuel-air mixture is compressed to a temperature and pressure at which it auto-ignites. HCCI engines have the potential for higher efficiency and lower engine-out pollutant emissions compared to more conventional spark-ignition or diesel engines. The autoignition process depends on chemical kinetics that occurs at relatively low temperatures and is highly sensitive to small variations in mixture composition and temperature.

The second model is based on two-zone heat release model to predict brake specific fuel consumption as well as volumetric emissions the inpust are the Engine cylinder Geometry , angles and the Temperature.

A. <u>The Numerical Modeling of Internal Combustion Engines with application to Simulation of combustion of single-cylinder HCCI engine by Cantera</u>

Details and Research Methodology

(HCCI) engine combines the best features of both Spark Ignition (SI)and Compression Ignition (CI)engines, offering a relatively high efficiency with low Nitrogen Oxides (NOx) and Particulate Matter (PM) emissions . The homogeneous mixture is achieved without using spark plug or injector to control its combustion phasing. Due to the absence of additional equipment to regulate its start of combustion, an HCCI engine does not typically give large gradients of spatial temperature from the flame front. As a result, it can significantly reduce NOx emissions. Moreover, since the mixture is premixed and very lean, it creates homogeneous charges inside the cylinder thus reducing the PM emissions significantly. In addition to its low emissions characteristic, an HCCI engine can also be operated at high compression ratio, producing more power and achieving higher efficiency compared to conventional engines.

However, despite its benefits in terms of high performance and low emissions, the combustion of HCCI engine is difficult to control. Moreover, to be widely used as a commercial engine, the HCCI technology has still a number of challenges to be solved. These include narrow operating range and the difficulty to regulate its heat release rate. It is also important to note that as the mixtures between air and fuel ignite nearly simultaneously at multiple location within the cylinder, knocking and misfire phenomena may occur. Therefore, controlling the combustion phasing remains the biggest challenge in HCCI combustion

In fact, the in-cylinder mixture in a piston engine is never perfectly homogeneous. Even if one started with a spatially uniform temperature and composition at intake-value closure, the temperature would become nonhomogeneous during compression as a result of wall heat transfer. Nevertheless, as a first approximation we will assume that the in-cylinder mixture remains homogeneous through the compression, autoignition, and expansion process. Moreover, we will assume that there is no heat transfer to or from the surroundings: all processes are adiabatic. These simplifications allow us to build a relatively simple model for a HCCI engine using a Cantera zero-dimensional reactor network.

To accurately represent the autoignition process, a sufficiently detailed reaction mechanism is required. Here we will us the same n-heptane mechanism .

To understand the use of n-heptane in HCCI engine for a wide range of operating conditions, varying some engine parameters such as air-fuel ratio (AFR), compression ratio (CR) and intake air temperature were needed. Firstly, the value of AFR was varied between 30 and 50, while intake air temperature, pressure, CR, and engine speed were kept constant. Afterwards, the value of CR was varied between 10 and 16. Lastly, the intake air temperature was varied between 300 and 360 K, while other engine parameters such as AFR, CR, and engine speed were kept constant.

Cantera model

We consider the time evolution of a closed (fixed-mass) homogeneous chemically reacting mixture with prescribed initial temperature, pressure, and composition, subjected to an imposed time-varying volume, and with no heat transfer to or from its surroundings (adiabatic).

We build an appropriate model using tools that are available in Cantera zero-dimensional reactor networks. We can simulate a homogeneous fixed-mass reactor with a specified time-varying volume by adding one additional component to our reactor network.

For this purpose, we use Cantera's object. A wall is defined as an interface between two Cantera Reactor() objects. A Reservoir is essentially a Reactor whose temperature, pressure, and composition remain fixed at their initial values.

Specifically, we define a Reservoir that contains ambient air, an Ideal Gas Reactor that corresponds to the homogeneous gas mixture in the combustion chamber of a piston engine, and a Wall representing a moving piston that separates the contents of the reservoir from those in the reactor. We prescribe initial conditions for the Reactor that correspond to the in-cylinder mixture temperature, pressure, and composition at intake-valve closure. We then move the Wall in a manner that causes the volume of the Reactor to vary in time as desired, and we monitor the time evolution of the temperature, pressure, and composition of the gas mixture in the Ideal Gas Reactor. Here we consider n-heptane/air initial mixtures

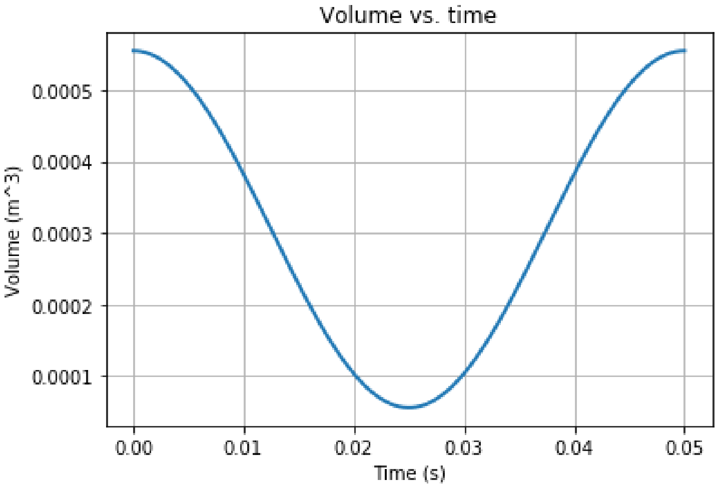
The HCCI we consider is a single cylinder of an automotive-size piston engine: a right-circular cylinder volume with a diameter of 86 mm, 86 mm (the piston *stroke s*s) over an engine cycle

We initialize the calculation with a fuel-lean fuel-air mixture at the maximum volume (assumed post-intake-valve closure conditions), and compute through one compression-expansion cycle (before exhaust-valve opening).

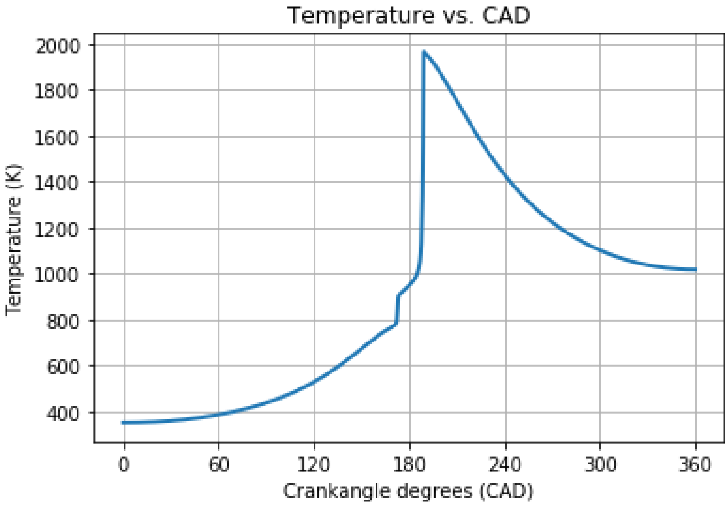
Results

- Volume Versus Time at defined Temperature

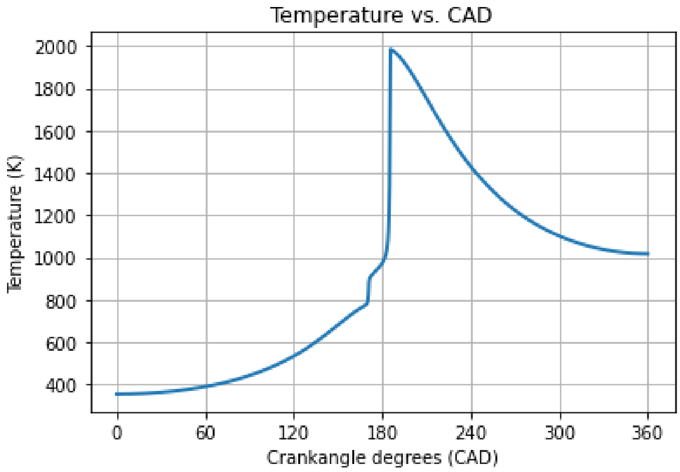
Temperature 350 K



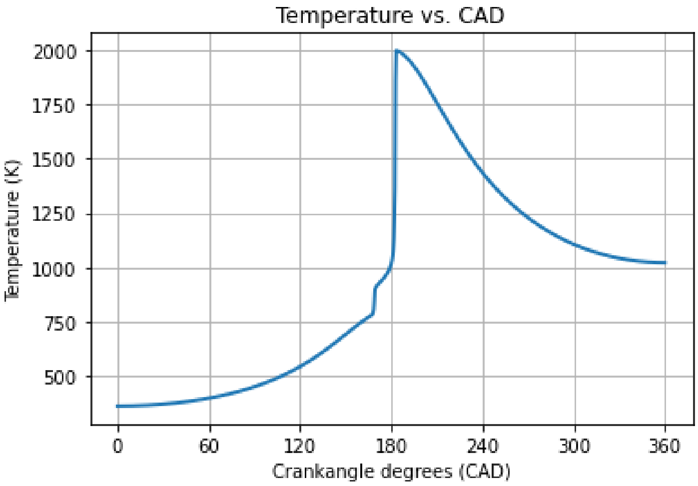
- Temperature Versus Crank degrees at defined compression ratio & Equivalence ratio & Temperature



CR=10
Phi=0.4
T=350K

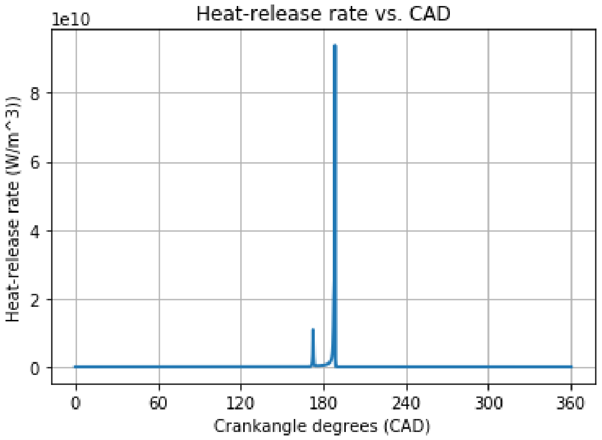


CR=10
Phi=0.4
T=355K

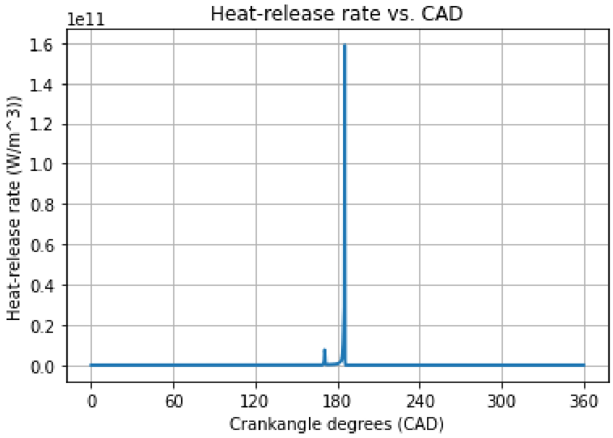


CR=10
Phi=0.4
T=360K

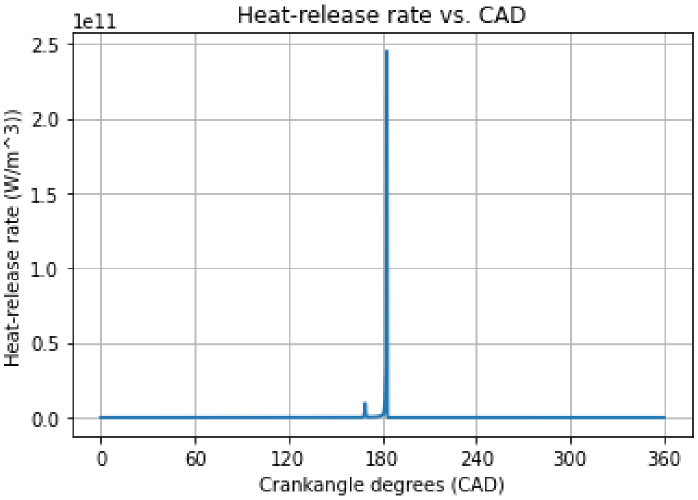
- Heat Release Versus Crank degrees at defined compression ratio & Equivalence ratio & Temperature



CR=10
Phi=0.4
T=350K

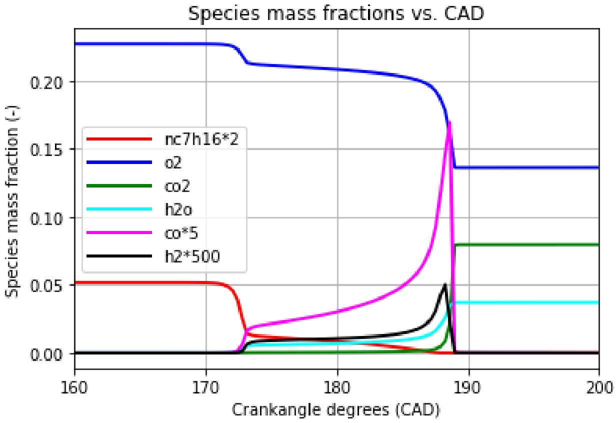


CR=10
Phi=0.4
T=355K

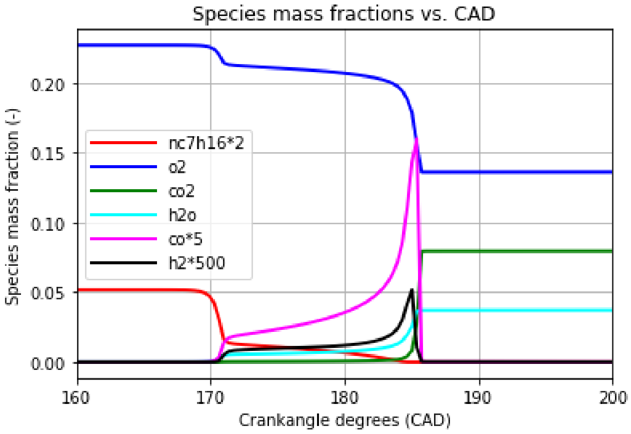


CR=10
Phi=0.4
T=360K

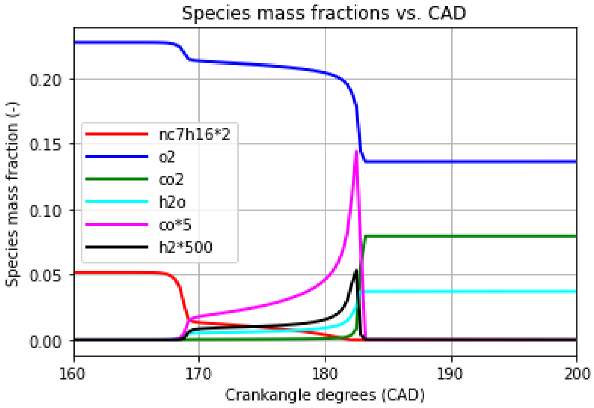
- Species mass fractions Versus Crank degrees at defined compression ratio & Equivalence ratio & Temperature



CR=10
Phi=0.4
T=350K



CR=10
Phi=0.4
T=355K



CR=10
Phi=0.4
T=360K

B. Application of Implementation of an Integrative MATLAB Engine Model and Validation on Waukesha VHP Series Engines

Details and Research Methodology

The MATLAB code Developed in University of Idaho to Model Spark Ignited Engines can accept basic input parameters such as bore, stroke, compression ratio, spark advance, throttle position, RPM, air/fuel equivalence ratio, Fuel Heating Values . In addition to power and torque predictions, the model described here uses a two-zone heat release model to predict brake specific fuel consumption as well as volumetric emissions. The simulations produced power and torque results very close to the actual outputs of the engine based on factory engine data. These simulations also yield brake specific fuel consumption and brake specific emissions maps that agree with empirical data.

The Model had been used to model the New VH P9394GSI S5 to its existing Waukesha VHP Series Five family of rich-burn gas engines, which includes the L7042GSI S5 at 1,500 HP and L7044GSI S5 at 1,900 HP. The major benefits of the Series Five family include up to 13 percent more power, better fuel flexibility and ambient temperature tolerance, up to 10 percent lower fuel consumption, up to 22 percent lower life cycle costs and longer service intervals than previous versions. That is achieved thorough improvement in design A modified cylinder head design reduces temperatures in key regions, thus extending the life of the cylinder head. Additionally, the piston design has also been enhanced, which helped reduce unburned hydrocarbons and the temperature of the and Finally Combustion efficiency.

The Engine Modeled Parameters

The Engine Parameters are

Stroke : 216 mm

Bore : 238 mm

Compression Ratio : 9.7 : 1

Fuel : Propane

The Engine is Supercharged Intercooled “GSI”

The Gravimetric Air to Fuel ratio is 15.6

The Molar Air to Fuel Ratio is 23.6

Combustion Burn Duration [degrees]=85

Crank Angle At Start of Combustion [degrees]=145

Time [degrees] when Intake Valve Closes =0

Time [degrees] when Exhaust Valve Opens=314

The Heating Value of Fuel =46.8e6 Joule/KG

Fraction Turbo charge considered of 250% Pressure Raise

Combustion Efficiency 90 %

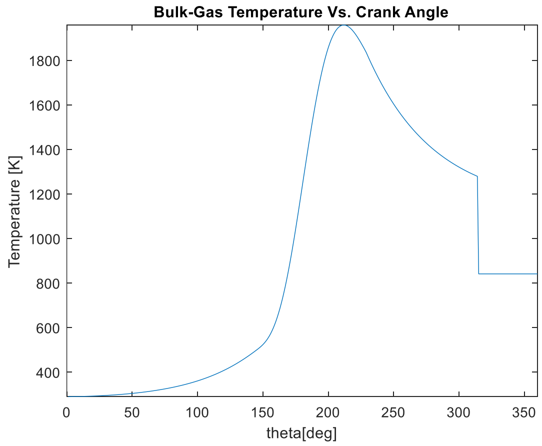
Air to Fuel Ratio Calculations

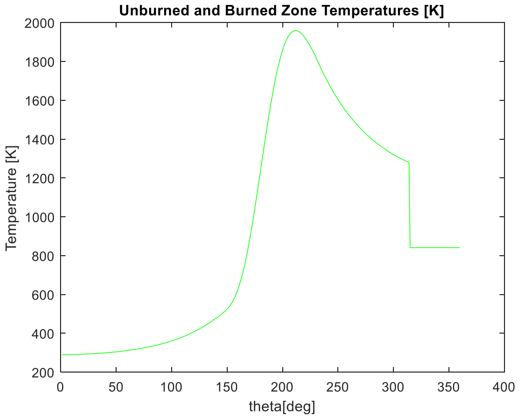
$C_3H_8 + 5 (O_2+3.76 N_2)$--------------$3 CO_2+4H_2O+18.8N_2$

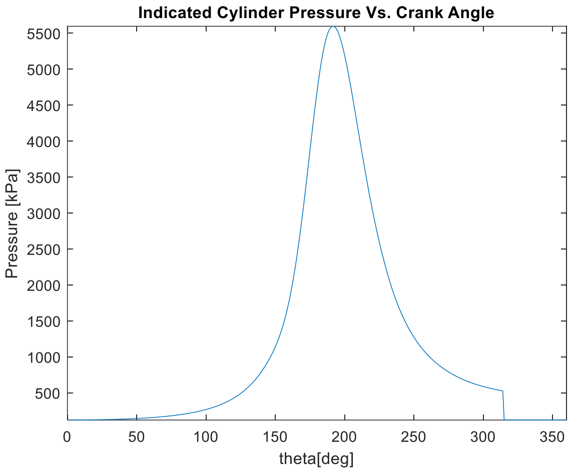
Gravimetric Air to fuel Ratio 5 x 4.76x29/(12x3+8)=15.6

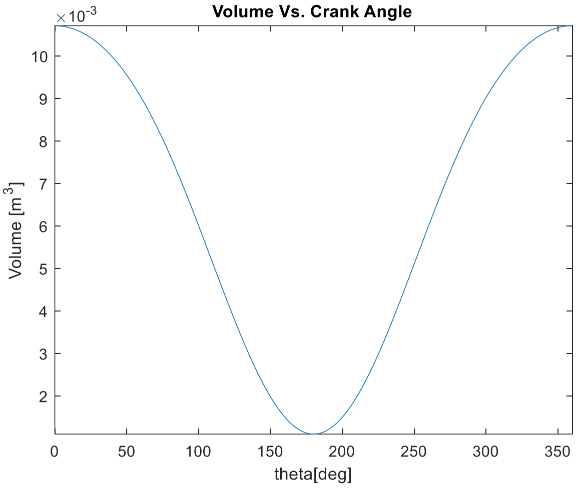
Molar Air to Fuel Ratio = 5x4.76/1=23.8

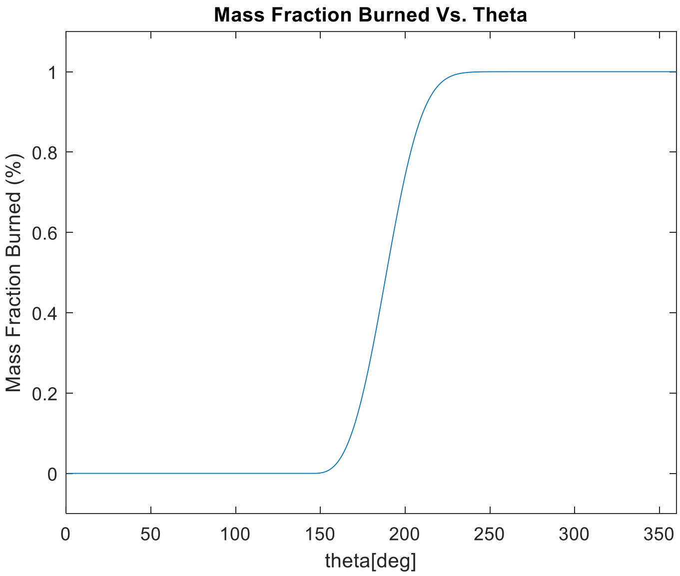
Results at 1000RPM











The Second Step will be to Run the Engine on Different RPMs and compare the same to catalogue data

RPM	Calculated Break Power KW	Catalogue Break Power KW
1000	1320	1327
900	1157	1193
1200	1663	1592

Conclusion

The Cantera Model could give a detailed study of the HCCI Engines & could be an interesting enhancer to the performance of Engine identifying the combustion characteristics with different parameters like the air fuel ratio and compression ratio and Inlet Temperature. The characteristics of combustion could be studied with the crank angle and the quantum of heat release could be also studied .The composition of the burned gases could be also studied thoroughly. The Cantera tool could be utilized in different combinations to enhance the performance of HCCI Engine and decrease emissions.

The Matlab code Had given within 5 % accuracy of the power generated at different RPMs of the Waukesha Gas Engine which indicates an excellent method of production performance

References

1. J. Heywood, Internal Combustion Engine Fundamentals. Tata Mcgraw Hill Education, 2011.
2. MathWorks MATLAB https://www.mathworks.com/products/matlab.html
3. Cantera https://cantera.org/

4. https://www.python.org/
5. C. Ferguson, and A. Kirkpatrick, Internal Combustion Engines: Applied Thermosciences. Third Edition. John Wiley & Sons, 2016.
6. Cuddihy, Jeremy. “A User-Friendly, Two-Zone Heat Release Model for Predicting Spark-Ignition Engine Performance and Emission”, MS Thesis, University of Idaho, 2014.
7. Cuddihy, J., Beyerlein, S., White, T., and Cordon, D., "MATLAB® Modeling of an IC Engine as a Capstone Learning Experience in a Combustion Engines Course," SAE Technical Paper 2016-01-0173, 2016, doi:10.4271/2016-01-0173.
8. Steven Beyerlein Theron White , Implementation of an Integrative MATLAB Engine Model as a Final Project in an Internal Combustion Engines Course
9. Stephen R. Turns AN INTRODUCTION TO COMBUSTION Concepts and Applications third edition
10. Zhao, F., Asmus, T. W., Assanis, D. N., Dec, J. E., Eng, J. E., and Najt, P. M. (eds.), Homogeneous Charge Compression Ignition (HCCI) Engines: Key Research and Development Issues, PT-94, Society of Automotive Engineers, Inc., Warrendale, PA, 2003.
11. A. Aziz Hairuddin1*, Talal Yusaf2 and Andrew P. Wandel3 Single-zone zero-dimensional model study for diesel-fuelled homogeneous charge compression ignition (HCCI) engines using Cantera
12. Janhunen TT. HCCI-combustion in the Z engine. SAE Technical Paper; 2012.
13. Automotive and Mechanical Engineering. 2013;8:1292. [2] Hasan M, Rahman M, Kadirgama K. A review on homogeneous charge compression ignition engine performance using biodiesel-diesel blend as a fuel. International Journal of Automotive and Mechanical Engineering. 2015;11:2199.
14. Najt PM, Foster DE. Compression-ignited homogeneous charge combustion. SAE Technical paper; 1983.
15. Jun D, Ishii K, Iida N. Autoignition and Combustion of Natural Gas in a 4 Stroke HCCI Engine. JSME International Journal Series B Fluids and Thermal Engineering. 2003;46:60-7.
16. Kong S-C, Reitz RD. Numerical study of premixed HCCI engine combustion and its sensitivity to computational mesh and model uncertainties. Combustion Theory and Modelling. 2003;7:417-33.
17. Nathan SS, Mallikarjuna J, Ramesh A. An experimental study of the biogas–diesel HCCI mode of engine operation. Energy Conversion and Management. 2010;51:1347-53.
18. Waukesha Gas Engines Catalogue
19. · Warstial Gas Engines Catalogue
20. · Caterpillar CHP units Catalogue