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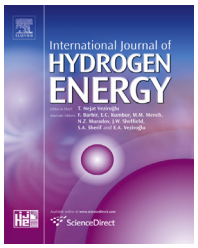

Development of chemical kinetics based hydrogen HCCI combustion model for parametric investigation

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ABSTRACT

Development of low pollution combustion technologies for internal combustion engines has become a major thrust area due to increase in air pollution from engine exhaust emissions. Homogeneous charge compression ignition (HCCI) combustion technology for internal combustion engines promises efficient combustion and cleaner emissions. HCCI engines can be run using multiple fuels such as gasoline, diesel, DME and hydrogen. Due to chemical kinetic nature of combustion in this engine, its combustion control is a major challenge. Using hydrogen as fuel can be a useful way to reduce emissions and improve combustion of HCCI engine. In the present work a stochastic multi zone chemical kinetics based model is developed to perform a parametric analysis on hydrogen HCCI engine. The model was validated against experimental results of HCCI engine run using hydrogen as fuel. Further, parametric studies were performed on the hydrogen HCCI engine using this model. Investigated parameters were equivalence ratio, intake temperature and charge quality. The parametric investigation is done to study the effect of these parameters on combustion and its control. The model is also used to predict the emissions of NO_x at these varying parameters. Effectiveness of charge dilution using CO_2 and H_2O in controlling the start of combustion has been examined. There was a noticeable agreement between the experimental results and simulated values. The parameters investigated show promising results, which can help in better control of ignition timings in hydrogen fuelled HCCI engine.

Introduction

In past few decades, the emerging trends of shifting seasonal patterns, broadened extremities of climate, rising sea level, increased toxicity of air in metropolitan areas and ever decreasing reserves of oil have made everyone conscious of global warming, emissions and sustainability. This has forced the mankind to look for alternative cleaner and renewable resources of energy. All the major economies of the world have formulated road maps for emission reduction and invested considerably huge amount of resources for search cleaner fuels and technologies. Hydrogen is one such highly sought after sustainable renewable resource. The integration of this hydrogen based solution with the current transport infrastructure is a necessity. Hydrogen combustion doesn't

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produce incomplete combustion products like CO and HC as emissions but NO_x produced is still a problem due to high temperatures produced during combustion in conventional engines [1,2]. Homogenised charge compressed ignition (HCCI) has shown great prospects as a technological upgrade to internal combustion engines by bridging gap between compression ignition and spark ignition technologies [3,4]. HCCI engines operate on a premixed fuel and the resulting combustion gas temperature is relatively lower. This combustion technology if used, with hydrogen and its blends with other fuels could show great promise in meeting the strict emission standards because HC emissions are major pollutant of concern from HCCI engines [5,6].

HCCI engine's biggest holding back factor is inability to control the combustion process directly as combustion is not initiated by a spark or injection but rather due to chemical kinetics of the mixture. HCCI combustion is suggested to be governed by the temperature and pressure conditions of the charge, which are the activation factors for the chemical kinetics [7,8]. This makes the control of process difficult under varying load and equivalence ratio. Wide flammability limits of hydrogen allows it to burn under different equivalence ratios, this could allow better control over combustion process. The factors that could help in controlling the combustion process are compression ratio, intake temperature, valve timings, equivalence ratio and quality of charge [9].

This paper presents a computational model with focus on speed at relatively low loss of accuracy for faster prediction of combustion characteristics on variation of key engine parameters. The model is tuned using experimental data published by Mohamed Ibrahim et al., 2014, which investigates into effects of charge dilution in hydrogen HCCI [10]. The accuracy of model is displayed by comparing pressure crank angle diagram and NO_x emissions. The parameters varied in the study are Intake charge temperature, equivalence ratio and charge quality (reduced by CO_2 and H_2O dilution).

Model details

Quasi-dimensional multi-zone model with detailed chemistry is developed using cantera, an open-source chemical kinetic code. These multiple zones are modelled to describe process in closed part of combustion i.e. after IVC and before EVO. The developed model is ''balloon-type'' quasi-dimensional multi-zone combustion model, as described by Kodavasal et al., 2013 [11]. The contents of the engine cylinder are modelled as multiple perfectly stirred reactors (PSR), which are deformable but with fixed mass. No heat or mass transfer occurs between the zones and pressure is maintained constant for all the reactors. The model uses hybrid approach as described by Aceves et al., 2001, where temperature profiles in different zones are specified until chemistry comes to play. These specified temperature profiles were obtained using CFD analysis of cylinder flow and compression process. The indirect coupling allows for faster solution as fluid mechanics equations are not solved along with chemical kinetics. This is particularly suitable for HCCI as combustion is dominated by chemical kinetics [12,13]. The reactors represent the thermal stratification and determine the burn duration and pressure rise rate, as the reactors undergo sequential auto-ignition. The flow diagram in Fig. 1 explains the working of model.

Description of zones and geometry

The Zones are divided into computational control volumes based on mass fraction decided by IVC volume of zones. These fractions represent three key regions inside the combustion chamber namely, the crevice, the boundary layer and adiabatic core. Each of the zone is represented in the code by a PSR with shared boundary, which is based on the assumption that charge temperature and composition is same throughout the cylinder at IVC timing. Only compression work is allowed to be transferred through boundary. Mass summation of all the zones remains constant throughout the run of the model but the volume of zone can change. The number of zones is defined by user based on a number that could best define the thermal stratification inside the cylinder.

$$\sum_{i=0}^{N} m_i = m_{total} \tag{1}$$

In equation (1), m_i is the mass inside 'ith' *zone* and 'N' represents the number of zones.

Heat transfer model

Heat is lost from the zones to the solid cylinder walls during the compression and expansion cycle. The heat loss is calculated at each point in time according to convective heat transfer equation (2).

$$Q_{wall} = hA(T - T_{wall}) \tag{2}$$

Where T_{wall} is the cylinder wall temperature, T is the temperature at instance calculated by assuming charge as air, A is the surface area of the volume of the reactor and the heat transfer coefficient, h, is obtained from equation (3).

$$Nu_h = aRe^b Pr^c \tag{3}$$

Where Nu_h is the Nusselt Number given by hL/k(where $h$is the convective heat transfer coefficient of the flow, L is the characteristic length, $k$is the thermal conductivity of the fluid), Re

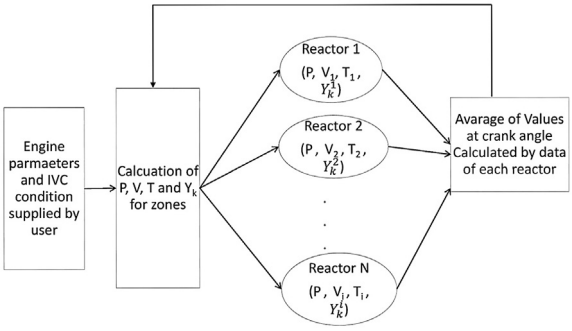

Fig. 1 – Reactors interactions with user specified parameters. After calculating Average values at each crank angle, the reactors are reinitialized with new values. Reactors solve only ideal gas law equations until crank angle to energy equation specifies.