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Mathematical modeling on the effect of equivalence ratio in emission characteristics of compression ignition engine with hydrogen substitution

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ABSTRACT

The investigation presented in this paper concerns on the computational simulation of emissions characteristics in compression ignition engine with hydrogen substitution. Combustion process has been modeled based on Equilibrium Constants Method (ECM) with MATLAB program to calculate the mole fractions of 18 combustion products when hydrogen is burnt along with diesel fuel at variable equivalence ratios. It can be observed that hydrogen substitution causes significant increase in NH_3, H_2, atom H emissions during rich combustion and OH, NO_2, HNO_3 emissions during lean combustion. As the equivalence ratio increases during rich combustion, mole fractions of HCN, CH_4, CO and atom C decreases with increment of hydrogen substitution. N_2, atom N and CO_2 emissions decrease whereas no significant changes in O_2, NO, O_3 and atom O emissions throughout all equivalence ratios as hydrogen is added to the combustion.

1. Introduction

In recent days, the importance of environment and energy are emphasized in various energy schemes. The stringent environmental regulations on exhaust emissions and anticipation of the future depletion of worldwide petroleum reserves provide strong encouragement for the research on alternative fuels. Hydrogen is one of the most promising alternative fuels. Its clean burning characteristics and better performance, drives more interest in using hydrogen fuel as an alternative fuel. Hydrogen, as an energy medium, has some distinct benefits for its high efficiency and convenience in storage, transportation and conversion. Hydrogen has been used widely in electricity generation, vehicle engines and aerospace [1]. The most important advantage of the hydrogen engine is that it emits fewer pollutants than other engines. Hydrogen offers a possible solution to such problems as energy security, resource availability and environmental concerns. It has the potential to be carbon-free source, unless produced from hydrocarbons.

Many researchers have used hydrogen as a fuel in a spark ignition (SI) engine. A significant reduction in power output was observed while using hydrogen in SI engine due to pre-ignition, backfire, and knocking problems at high load. These problems cause the usage of hydrogen fuel in a SI engine only within a limited operation range [2]. However, hydrogen cannot be used as a sole fuel in a compression ignition (CI) engine, since the compression temperature is not enough to initiate the combustion due to its higher self-ignition temperature [3]. Hence, an ignition source is required while using it in a CI engine. The simplest method of using hydrogen in a CI engine is to run in the dual fuel mode with diesel as the main fuel that can act as an ignition source for hydrogen. In a dual fuel engine, the main fuel is either carbureted or injected into the intake air

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Nomenclature

NO	nitrogen oxide
CO	carbon monoxide
CO_2	carbon dioxide
HC	hydrocarbon
H	atom hydrogen
H_2O	water
O_2	oxygen
NH_3	ammonia
HCN	hydrogen cyanide
OH	hydroxide
ECM	Equilibrium Constant Method
LTCM	Low Temperature Combustion Model Method
H_2	hydrogen gas
N	atom nitrogen
HNO_3	nitric acid
O_3	tri-oxygen
CH_4	methane gas
C	atom carbon
N_2	nitrogen gas
NO_2	nitrogen dioxide

stream with combustion initiated by diesel. The major combustion energy is obtained from diesel while the rest of the combustion energy is supplied by hydrogen.

Most of the research in hydrogen dual fuel CI engine focused on experimental study of performance and emissions. Karim [4,5] concluded that at low loads, much of the primary gaseous fuel remains unburnt leading to high hydrocarbon (HC) and carbon monoxide (CO) emissions. At high loads, a large amount of gaseous fuel admission results in uncontrolled reaction rates near the pilot spray causing rough engine operation. Shidfar and Garshasbi developed a combustion mathematical model for measuring cylinder pressure in a combustion engine [6]. Bahadir and Ellerby [7] studied the combustion process of the in situ combustion simulator and Liu [8] determined the key factors to reduce carbon dioxide (CO_2) emissions from combustion.

In the present study, an effort is made by developing a combustion mathematical model to simulate exhaust emissions in hydrogen–diesel blend fuels. Based on Equilibrium Constants Method (ECM), a computer program using MATLAB has been developed for the blended fuels to calculate the mole fractions of the emission gases. ECM is based on thermodynamic measurements and empirical calculations. It is very accurate and precise in solving most of chemical kinetics problems [9]. Thermodynamic data for elements, combustion products and many pollutants are available in a compilation published by the National Bureau of Standards, called the JANAF (Joint Army–Navy–Air Force) tables. The equilibrium constant data from JANAF tables using polynomial curve fitted has been used in calculating the combustion products [10].

2. Combustion modeling approach

In this study, the derivations of governing equations for the reaction combustion equations were performed by assuming 18 combustion products. A system of 19 nonlinear equations appears in the derivation of the reaction combustion equations and it can be solved using Newton–Raphson methods prior to its implementation into MATLAB program.

2.1. Governing equations

Combustion of hydrocarbon fuels at low temperature produces N_2, H_2O, CO_2 and O_2 for lean mixtures ($\phi < 1$) and N_2, H_2O, CO_2, CO and H_2 for rich mixtures ($\phi > 1$). At higher temperatures (usually above 1600 K), these major species dissociates and react to form additional species with significant amounts [11]. By considering these phenomena and assuming 18 combustion products, the reaction combustion equations for hydrocarbon–hydrogen blend fuels with air can be written as:

$$n_f C_\alpha H_\beta + pH_2 + \frac{a_s}{\varphi}(O_2 + 3.76N_2) \rightarrow n_T[y_1H_2 + y_2H_2O + y_3CO_2 + y_4N_2 + y_5O + y_6O_2 + y_7O_3 + y_8H + y_9OH + y_{10}CO + y_{11}C + y_{12}CH_4 + y_{13}NO + y_{14}NO_2 + y_{15}NH_3 + y_{16}HNO_3 + y_{17}HCN + y_{18}N]. \quad (1)$$