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# Investigation on Effects of Water Addition on Performance and Emissions of an n-heptane Fueled Homogeneous Charge Compression Ignition Engine

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ABSTRACT: The main purpose of current study is investigation on the effect of water addition on n-heptane homogenous charge compression ignition combustion. A multi zone model coupled to the semi-detailed chemical kinetics mechanism is used for simulation of n-heptane homogenous charge compression ignition combustion. First, the accuracy of the model was estimated for two different operating modes, and then seven different amounts of water were added to the fuel and its effects on n-heptane combustion were investigated. Thermal, chemical and dilution effects of water are studied using artificial inert species method. The results show that the start of combustion was retarded by water addition due to the thermal effect of water. Peak values of in-cylinder pressure and heat release rate decreases by water addition. Water addition has caused the maximum amount of radicals in the combustion chamber to be reduced and the time of their formation is delayed. Water addition increases the amount of unburned hydrocarbons at exhaust. Thermal effect of water on start of combustion and emissions formation is more significant than its dilution and chemical effects. Using small quantities of water will increase the thermal efficiency of the engine and reduce emissions from it.

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## 1. Introduction

The Homogeneous Charge Compression Ignition (HCCI) engines have low exhaust NOx and fuel consumption and significant power. Of course, these engines also have disadvantages that have prevented their commercialization for dynamic applications. The main disadvantages of these engines is the lack of a means for direct control of them [1-3]. One of the ways to control combustion in HCCI engines is to use additives. Additives are combinations that combine fuel and air inside the combustion chamber, and control the combustion with a change in mass percentages [4,5]. There are several other add-ons that have been frequently studied in literature [6-8]. Water vapor is one of the additives that can be used by internal combustion engines. With the idea of HCCI engines, the idea of adding water to combustion components in these engines has also been considered.

# 2-Methodology

In this study, a multi-zone model is used to simulate the engine closed cycle. The combustion chamber is divided into four general types: the core zone, the middle zones, the boundary layer zone, and the crevice zone. The boundary layer zone is the nearest zone to the wall and is exchanging heat with the wall. The equations of the first law of thermodynamics and chemical kinetics are solved simultaneously for each zone at each time step. Eqs. (1) to (5)show the governing equations.

$$\frac{dU_i}{dt} = -\frac{dW_i}{dt} + \frac{dQ_i}{dt} \tag{1}$$

$$\frac{dU_{i}}{dt} = c_{v}^{i} m_{i} \frac{dT_{i}}{dt} + m_{i} \sum_{j=1}^{n_{i}} u_{j} \frac{dY_{j}}{dt} + \sum_{j=1}^{n_{i}} u_{j} Y_{j} \frac{dm_{i}}{dt}$$
(2)

$$\frac{dW_i}{dt} = P \frac{dV_i}{dt} \tag{3}$$

$$\frac{dQ_i}{dt} = \frac{dQ_{i,cond}}{dt} + \frac{dQ_{i,conv}}{dt} + \frac{dQ_{i,mtran}}{dt}$$
(4)

$$\frac{dY_{k,i}}{dt} = \frac{\dot{\omega}_{k,i}Mw_k}{\rho} \tag{5}$$

Further details of the model and are available in previously published studies [9,10]. The combustion process of n-heptane is simulated utilizing a chemical kinetics mechanism containing 57 species and 290 reactions [11]. Seven different amounts of water are added to the fuel and effects of water on n-heptane HCCI combustion are focused.

### **3-Discussion and Results**

Two different operating modes have been selected and the effects of water addition on them have been investigated. Table 1 shows the characteristics of the two cases.

For validation of the model, experimental data of the Cooperative Fuel Research (CFR) engine available at the University of Alberta has been used. Experimental and

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Case	Rc	λ	Exhaust gas	Engine
number			recirculation	speed
			(%)	(rpm)
1	12.7	3.87	0	700
2	12.7	2.46	40	700

**Table 1. Engine operating conditions** 





Fig. 1. Experimental and numerical curves for the in-cylinder pressure

numerical in-cylinder pressure curves are indicated in Fig. 1. Table 2 also shows the data on engine emissions for both of the cases. As the figure and table show, the model has a good accuracy in prediction of the in-cylinder pressure and exhaust emissions.

After verifying the model, seven different amounts of water are added to the in-cylinder mixture and its effects on n-heptane combustion are studied. Fig. 2 shows the effects of the water addition on the in-cylinder pressure. As shown in this figure, with the addition of water, the peak pressure decreases and its position is delayed. This is because water is a tri-atom molecule with a high specific heat capacity, so it absorbs the heat of the combustion chamber and reduces the in-cylinder temperature and causes delayed chemical reactions. With the delay in the initiation of reactions, the

Table 2. Numerical (Num.) and Experimental (Exp.) values of engine exhaust emissions

engine exhaust emissions									
Case	Exp.	Num.	Exp.	Num.	Exp.	Num.			
number	$CO_2$	$CO_2$	CO	CO	UHC	UHC			
А	3.71	3.71	0.073	0.073	995	867			
В	6.33	6.32	0.149	0.148	1705	1573			



Fig. 2. Effect of water on in-cylinder pressure and temperature of core zone

main stage of heat release is transferred to the expansion process, which prevents significant pressure increase and reduces the peak pressure.

#### 4-Conclusion

In the present study, water has been added to the HCCI engine –n-cylinder mixture and its effects on the performance and pollutants of engine have been investigated. HCCI engine is simulated utilizing a thermodynamic multi zone model. A semi-detailed chemical kinetics mechanism is applied for combustion process modelling. Seven different values of water are added to in-cylinder mixture and its various effects are studied. The most important results are:

Use of water delays the start of combustion.

• Water addition reduces in-cylinder pressure and temperature.

• Using small quantities of water will increase the thermal efficiency of the engine and reduce exhaust emissions.

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