Energy Proceedings Vol 27, 2022

Supercritical fuel combustion in a compression ignition engine cylinder

Zhichao Zhang ^{1*}, Yiji Lu ², Yaodong Wang ³, Tony Roskilly ³

1 Department of Mechanical and Construction Engineering, Northumbria University, Newcastle upon Tyne, NE1 8ST, UK

2 James Watt School of Engineering, University of Glasgow, Glasgow, G12 8QQ, United Kingdom

3 Durham Energy Institute, Durham University, Durham, DH1 3LE, United Kingdom

ABSTRACT

In this paper, the supercritical (SC) fuel combustion is investigated on its performance in a diesel engine cylinder to improve output power and reduce emissions. The computational fluid dynamics (CFD) model is developed to comparatively study the spray combustion and the SC fuel combustion in a cylinder during constant volume combustion period. Results indicate that the engine in-cylinder pressure and output power can be increased by 6.8% and no less than 2.5% respectively. Moreover, the fuel concentration and temperature field of the SC combustion are more evenly distributed, which enables more sufficient combustion and indicates the potential to reduce pollutants such as NO_x and soot.

Keywords: clean combustion, supercritical fuel, compression ignition engine, computational fluid dynamics

NONMENCLATURE

Abbreviations	
CFD	Computational fluid dynamics
CI	Compression ignition
DF	Diesel fuel
SC	Supercritical

1. INTRODUCTION

Conventional spray combustion in compression ignition (CI) engines has shortcomings such as lower engine efficiency, incomplete combustion and less desirable exhaust emissions, especially NO_x and soot in CI engine cylinders [1]. Some researchers [2, 3] added gas fuels of high energy density such as hydrogen to the diesel fuel (DF) for better combustion process. They found improved thermal efficiency, in-cylinder pressure and reduced CO, unburnt hydrocarbons (HC) and soot emissions at most engine conditions, but increased NO_x emissions with the addition of hydrogen. Alcohols such as ethanol and butanol were also employed in various studies [4, 5], and demonstrated higher thermal efficiency and less soot emissions to the combustion process of CI engines. However, reduced output power, higher fuel consumption, and increased HC and CO emissions were observed. Therefore, these solutions to improve the combustion process of CI engines struggle in the trade-off among thermal efficiency, output power, NO_x emissions and soot emissions.

Supercritical (SC) state is the state that the temperature and pressure of a fluid exceed the critical point. The fluid at SC state has high density like liquid, and its ultra-low surface tension results in no phase boundaries with other fluid [6, 7]. These characteristics enable the SC fuel to mix with air more sufficiently and does not need time and heat to break up and evaporate. Therefore, the SC fuel is another method to improve efficiency and reduce emissions.

The SC state of fuels were studied by several researchers. Lin et al. [8] calculated the thermal properties of various DF surrogates at SC state, which provided fundamental data for investigating SC fuel combustion. Anitescu et al.[7] studied the phase transition and thermal behaviour of DF with diluent and indicated that the Soave-Redlich-Kwong (SRK) equation of state (EOS) can describe the phase transition well. So far, no investigations were done on SC fuel combustion under the condition similar to CI engine cylinders. Therefore, this paper will investigate the SC combustion of DF and analyze its benefits to the combustion process and engine performance using the CFD modelling.

2. METHODOLOGY

2.1 Experimental system

The test rig is a Cummins ISB4.5 turbocharged diesel engine system. The layout of the test rig is shown in Fig. 1. The specifications of the engine are listed in Table 1. The engine is running at 1800 rpm speed and full load. Its in-cylinder pressure is measured by an AVL QC34C watercooled high-speed pressure transducer. An AVL 365C encoder is mounted on the crankshaft to record the crank angle degree. The engine is connected with an eddy-current W230 dynamometer. For the emissions, a Horiba MEXA 1600DEGR gas analyzer is employed to measure the NO_x, CO and hydrocarbon in the exhaust, whilst a Horiba SPCS 1000 measures particulate number.



Fig. 1. Layout of the engine test rig

Table 1. Engine specifications

Specification	Value	
Engine model	ISB 4.5	
Engine displacement (L)	4.5	
Compression ratio	17.2	
Length of connecting rod (mm)	192	
Holes on each injector	8	
Orifice of injection hole (mm)	0.167	
Number of cylinders	4	
Cylinder stroke length (mm)	124	
Cylinder bore (mm)	107	
MAX torque (N m)	760 at 1400 ~ 1800 rpm	
MAX power (kW)	152 at 2300 rpm	

2.2 Numerical model

Under the engine condition, the start of injection (SOI) and the peak in-cylinder pressure are at -5.47° TDC and 10.2° TDC. Therefore, the duration of this period is 1.45 ms and the movement of the piston in this period is 0.405 mm, which means the change in cylinder volume is neglectable. Accordingly, a 3D geometric model of 1/8 of the cylinder is built with the in-cylinder volume at SOI (0.0119L). The model is meshed using tetra/mixed unstructured mesh with the global size of 1.5 mm and refined to 0.02 mm at the zone near the injector, as shown in Fig. 2. The total amount of mesh is 315,167.

The fuel used in the experiment and the CFD models is DF. Its density is 835 kg/m³. The boundary conditions of the model are shown in Table 2 for the conventional spray combustion and SC fuel combustion respectively. The CFD models are run by ANSYS Fluent 18.1 for spray combustion and SC fuel combustion at the same condition as the engine from the SOI to the time of peak in-cylinder pressure (1.45 ms in total).

The Wave breakup model is selected for the droplets in the conventional spray combustion, which considers the breakup of the droplets to be induced by the relative velocity between the gas and liquid phases. It assumes that the Kelvin-Helmholtz instability dominates droplet breakup, and the size of child droplets is proportional to the wavelength of the unstable surface wave on the parent droplet [9].



Fig. 2. Meshed cylinder model (a) with refinement (b)

The non-premixed combustion model with the Probability Density Function (PDF) approach is selected for both conventional spray combustion and SC fuel combustion, because it is developed for turbulent diffusion flames with fast reactions. It assumes that the reaction chemistry is sufficiently rapid for equilibrium and thus enables turbulence-chemistry coupling [10].

In aforementioned context, the fuel at SC state has similar compressibility, viscosity and diffusivity to gas but liquid-level density. In the non-premixed combustion model, all materials participating in combustion are regarded as gas, which enables the viscosity and diffusivity of the fuel validated for its SC state. In terms of compressibility or density, the Soave-Redlich-Kwong (S-R-K) EOS is selected to describe fluids near and above their critical points. The equation is written as [11]:

	RT	а	(4)
p	$= \frac{1}{V-b}$	$\frac{1}{V^2+bV}$	(1)
		I	a shaka ta a dhuu a suu akta wa hadau u

Where a and b are obtained by equations below:

$$a = a_0 [1 + n(1 - (T/T_c)^{0.5})]^2$$
⁽²⁾

$$b = \frac{0.08664RT_c}{n_c}$$
(3)

Here a_0 and n are calculated by equation (4) and (5). $a_2 = \frac{0.42747R^2T_c^2}{(4)}$

$$P_0 = \frac{p_c}{p_c} \tag{4}$$

$$n = 0.48 + 1.574\omega - 0.176\omega^2 \tag{5}$$

Where T_c and p_c are the critical temperature and critical pressure respectively. ω is the acentric factor.

3. RESULTS AND DISCUSSION

3.1 Model validation

The in-cylinder pressure of spray combustion from the SOI to the peak pressure is obtained to validate the model against the experimental data.

Table 2.	Configuration	of initial	boundary	conditions /

Zone	Parameter		Value
	Fuel molar fraction		1
	N_2 and O_2 molar fractions		0
	Engl to management (W)	Spray combustion	312.85
Injector hole	Fuel temperature (K)	SC fuel combustion	730
5	Fuel mass flow (kg/s)		0.00819
	Fuel velocity (m/s)		447.79
	Fuel droplet size (mm)		0.167
	Luis stiens terms	Spray combustion	Droplets surface injection
SC f		SC fuel combustion	Mass flow inlet
	Fuel molar fraction		0
In-cylinder	N ₂ molar fraction		0.21
	O ₂ molar fraction		0.79
Zone	Temperature (K)		1175.68
	Pressure (bar)		126

As shown in Fig. 3, the predicted in-cylinder pressure agrees with the experimental data with the error no more than 1.4% at most time (0 ~ 1.1 ms). The error stays relatively stable before 1.1 ms but then increases to 7.1% at 1.45 ms, because the volume of cylinder after about 1.1 ms expands to larger than that at SOI, which reduces the in-cylinder pressure. It demonstrates that the CFD model can still predict the in-cylinder combustion of the CI engine from the SOI to the peak pressure.



Fig. 3. Predicted in-cylinder pressure of CDF model versus the experimental data for spray combustion

3.2 SC fuel combustion versus spray combustion

The in-cylinder pressure of SC fuel combustion from the SOI to the peak pressure is obtained and shown in Fig. 4, where the dash curves refer to the SC fuel combustion, and the solid curves are the conventional spray combustion. It demonstrates that the in-cylinder pressure of SC fuel combustion is higher than that of spray combustion at most time after the SOI. Moreover, the difference between them increases with time and finally reaches 12.3 bar at the peak pressure. The major reason is that the fuel at SC state is more sufficiently burnt due to more uniform fuel-air mixing process. Phenomenon is also likely to be caused by the heat loss during the conventional spray combustion, where liquid fuel droplets absorb heat from hot in-cylinder gas to evaporate, which does not exist in the SC fuel combustion. Therefore, the SC fuel combustion is likely to increase the engine output power.



Fig. 4. In-cylinder pressure of SC fuel combustion versus spray combustion

Fig. 5 illustrates the in-cylinder fuel distributions and temperature fields of the two different combustion method at the moment of peak in-cylinder pressure. Zone A is the fuel-lean zone in the two cases. However, during the spray combustion, the temperature of zone A is higher and the area of high temperature zone is larger than those during SC combustion. This phenomenon will promote NO_x formation in spray combustion according

to the thermal NO_x mechanism [10], which dominates

fuel-lean and high temperature conditions.



Fig. 5 Temperature fields and fuel distributions at 1.45 ms in spray combustion and SC fuel combustion

In the zone B, both the spray combustion and the SC fuel combustion are fuel-rich, but the temperature of zone B in the spray combustion is lower than that in the SC combustion, which promotes the Prompt NO_x formation. As a result, it can be predicted that the total NO_x emission in the spray combustion would be higher than that in the SC fuel combustion.

In zone C, the temperature of the SC fuel combustion is close to that of the spray combustion, but the fuel mass fraction there is much lower than that of the spray combustion. Consequently, more soot is likely to be generated by the spray combustion in zone C. Moreover, the high temperature area in zone C during the spray combustion is closer to the wall (piston bowl) compared to that during the SC fuel combustion, which is the seedbed for soot. Consequently, the situation in the SC combustion is less beneficial to soot formation.

4. CONCLUSIONS

In the paper, CFD models of the CI engine cylinder are developed to investigate the SC fuel combustion. This study demonstrates the SC fuel combustion has the potential to produce increased engine output power, more sufficient fuel combustion and more uniform incylinder temperature distribution, which may benefit to CI engines in terms of pollutant reduction.

ACKNOWLEDGEMENT

The authors would like to thank the support of EPSRC (EP/K503885/1) for the project 'Study of engine waste heat technologies' and the financial support of MCE QR fund (cc101103) from Northumbria University.

REFERENCE

[1] Yun H, Reitz RD. Combustion optimization in the lowtemperature diesel combustion regime. International Journal of Engine Research. 2005;6:513-24.

[2] An H, Yang W, Maghbouli A, Li J, Chou S, Chua K, et al. Numerical investigation on the combustion and emission characteristics of a hydrogen assisted biodiesel combustion in a diesel engine. Fuel. 2014;120:186-94.

[3] Zhou J, Cheung C, Leung CJAe. Combustion, performance, regulated and unregulated emissions of a diesel engine with hydrogen addition. 2014;126:1-12.

[4] Karthikeyan B, Srithar K. Performance characteristics of a glowplug assisted low heat rejection diesel engine using ethanol. Applied Energy. 2011;88:323-9.

[5] Zheng M, Han X, Asad U, Wang JJEc, management. Investigation of butanol-fuelled HCCI combustion on a high efficiency diesel engine. 2015;98:215-24.

[6] Wensing M, Vogel T, Götz G. Transition of diesel spray to a supercritical state under engine conditions. International Journal of Engine Research. 2016;17:108-19.

[7] Anitescu G, Tavlarides LL, Geana D. Phase transitions and thermal behavior of fuel- diluent mixtures. Energy & Fuels. 2009;23:3068-77.

[8] Lin R, Tavlarides LL. Thermophysical properties needed for the development of the supercritical diesel combustion technology: Evaluation of diesel fuel surrogate models. The Journal of Supercritical Fluids. 2012;71:136-46.

[9] Liu AB, Mather D, Reitz RD. Modeling the effects of drop drag and breakup on fuel sprays. DTIC Document; 1993.

[10] Ismail HM, Ng HK, Gan S. Evaluation of non-premixed combustion and fuel spray models for in-cylinder diesel engine simulation. Applied Energy. 2012;90:271-9.

[11] Soave G. Equilibrium constants from a modified Redlich-Kwong equation of state. Chemical engineering science. 1972;27:1197-203.