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THE 3-D SIMULATION WITH DETAILED CHEMICAL KINETICS OF THE TURBULENT COMBUSTION IN A PRE-CHAMBER INDIRECT INJECTION DIESEL ENGINE

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ABSTRACT

A 3-D CFD model based on KIVA 3 code is developed with a "reduced" detailed chemical kinetics of 291 elementary reaction steps with 79 chemical species for diesel fuel combustion. The model was validated by the corresponding experimental results and employed to examine some important parameters which have significant effects on the engine performance for an IDI diesel engine with a swirl chamber. It shows as an example that chamber surface temperature, nitrogen addition, liquid fuel spray cone angle, injection timing, and activated radicals in the residual gases can have significant effects on engine combustion and performance. The modeling approach has the potential to be employed for predicting and optimizing engine performance. Some apparent limitations of the model were identified and some potential remedial measures outlined.

NOMENCLATURE

ATDC after top dead centre
DI direct injection
IDI indirect injection
EGR exhaust gas recirculation
EQ equivalence ratio
n engine speed
NOx nitrogen oxides
P pressure
PSR perfectly stirred reactor
T temperature
TDC top dead centre

Subscripts

in intake

INTRODUCTION

The internal combustion engines will continue in the foreseeable future to play a major role in providing power for road vehicles and industrial plants. In order to satisfy the requirements of the ever stricter regulations for emissions worldwide, engines with swirl chambers have been widely used in transport and utility power applications due to their advantages of relatively low NO_x emissions, low noise, and good adaptability to changes in engine speed. However, to improve the specific fuel consumption and starting performance at low ambient temperature remain a challenge.

With the ever increasing speed and capacity of computing equipment, multidimensional modelling has become a feasible and economical tool in engine design and development processes (He and Rutland, 2002). Good computer modelling can be used for obtaining a better understanding of the complexities of the combustion process within engines, finding effective measures to overcome some operational problems, evaluating new design concepts, and reducing hardware prototype and development time and costs. Compared with the extensive research on the modelling of direct injection (DI) diesel engines (He and Rutland, 2002; Dong, 1996; Golovitchev et al., 2003), there are fewer references on the CFD simulation of indirect injection (IDI) diesel engines due to the increased complexity of both the geometry of the combustion chamber and the combustion processes involved (Giannattasio and Micheli, 1997; Ogawa et al., 1997; Liu, 2006). There is a need to develop a suitable 3-D CFD modelling with sufficiently detailed chemical kinetics to simulate the combustion processes of this kind of engines.

The present contribution, describes the results of a 3-D CFD model developed with a "reduced" detailed chemical kinetics of diesel fuel combustion in air, while considering the turbulence function for simulating the combustion processes of an IDI diesel engine with a swirl chamber. Experimental results were used to validate the model. Predicted features of the performance and combustion characteristics of the engine showed the influence of some changes in engine operating conditions including the chamber surface temperature, the presence of exhaust gas recirculation (EGR) or a diluent such as nitrogen in the intake air, and fuel injection spray characteristics. Relatively good agreement was demonstrated between predicted values and corresponding experimental results. Some apparent limitations of the model were identified and some potential remedial measures outlined.

MODEL DESCRIPTION

The Model

There are a number of commercial CFD-three dimensional program packages available on the market, including KIVA, which has been widely used for engine simulations. The original version of the model employed only global type combustion reaction kinetics. It needs to be suitably modified to simulate more reliably the details of the important complex chemical processes leading to autoignition and subsequent combustion. To do this

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suitably reduced detailed chemical kinetics for the fuel systems, including hydrogen, *n*-heptane and diesel fuel were incorporated into the modified code. The solving of the comprehensive kinetic scheme reaction rates equations with the perfectly stirred reactor (PSR) assumption will show the changes in the concentrations of the different species over the time increment represented by the corresponding residence time. Such calculated changes are entirely kinetically based. The use of kinetics-controlled reaction rates usually results in very fast combustion rates (Khalil and Karim, 2002). The fuel, oxidizer, and intermediate products may not have enough time then to mix down to the molecular level in the actual engine environment. Also, the presence of combustion products with the air-fuel mixture may result in the reactions to be partly controlled by the breakup of turbulent eddies that can produce correspondingly slower reaction rates.

Accordingly, both chemical kinetics and turbulence influence the course of the combustion processes in practical engines requiring suitable modeling of this interaction (Kong et al., 2001; Rente et al., 2001). Therefore, a turbulence-chemistry combustion model, based on a partially stirred combustion model, was developed and incorporated into the code.

A more realistic representation, which takes into account the additional contribution of turbulent mixing, considers that for a small incremental change in concentrations the corresponding time increment can be viewed to be made up of two segments: a chemical time increment on the basis of the perfectly stirred reactor assumption and a physical part due to the contribution of turbulent mixing effects.

Practical diesel fuels consist of a great number of compounds, mainly of the aliphatic and aromatic types. It is not possible at present to model its combustion reactions effectively using a sufficiently comprehensive chemical mechanism due to the very complex and varying combustion reactions of such compounds. A practical approach is to propose a surrogate fuel with a very few components of relatively known reaction schemes that can be used instead in the numerical simulations (Golovitchev et al., 2003). The aliphatic part of the diesel fuels can be represented by *n*-heptane (C_7H_{16}), since its cetane number is close to that of conventional diesel fuels, and its reaction kinetics can be simulated while the aromatic part of diesel fuel can be expressed by toluene (C_7H_8) of also relatively known kinetics. The overall equivalent molecule of the No. 2 diesel fuel was assumed to be approximated by $C_{14}H_{28}$ with its thermodynamic properties represented by polynomial functions. The detailed reduced chemical kinetic scheme of the fuel was validated and made up of 291 reactions and 79 species (Golovitchev et al., 2000; Golovitchev et al., 2003), which included the following overall reactions:

$$C_{14}H_{28} + 2H_2O \rightarrow 2C_7H_{16} + O_2 \quad (1)$$

$$C_{14}H_{28} + 3O_2 \rightarrow 2C_7H_8 + 6H_2O \quad (2)$$

When the reaction rates in Equation (1) and (2) are the same, the molar ratio of *n*-heptane to toluene is 75/25 since the reaction becomes:

$$2C_{14}H_{28} \rightarrow 3C_7H_{16} + C_7H_8 \quad (3)$$

There are chemical reaction atom conservation equations in the KIVA 3 code and the developed program in this contribution ensured throughout that the atom conservation for the different chemical reactions were satisfied. Moreover, since a sufficiently comprehensive chemical kinetics scheme was used to model the reactions activity in the engine, all phases of the combustion processes, including those associated with ignition, were predicted and no empirical model for ignition was needed (Karim, 2003). A more detailed description of the modeling approach can be found elsewhere (Liu and Karim, 2005; Liu et al., 2007).

Validation of the Model

An example of the mesh employed for the engine is shown in Figure 1. The engine is a three cylinder water-cooled, indirect injection Isuzu 3KC1 diesel engine. It has a compression ratio of 23:1, a 74 mm bore and 76 mm stroke. The mesh size was selected based on a compromise between accuracy and the time required to finish the calculation. The results of an experimental investigation of the diesel engine were reported by the present authors elsewhere recently (Xiao et al., 2009). The calculated and experimental cylinder pressure-time curves for an operational condition of a relatively large equivalence ratio of diesel fuel combustion are compared in Figure 2. The predicted pressure-time diagram displays generally good agreement with the experimental pressure development. It can be seen that the main difference between the calculated pressure results and the measured ones occurs mainly before Top Dead Centre (TDC) around the point when ignition occurs. This is probably caused by the fact that the simulated pressure is the calculated mean cylinder pressure while the measured one is the pressure which was indicated by the pressure transducer located in the swirl chamber. The measured result could not correspond exactly with the averaged mean pressure in the cylinder.

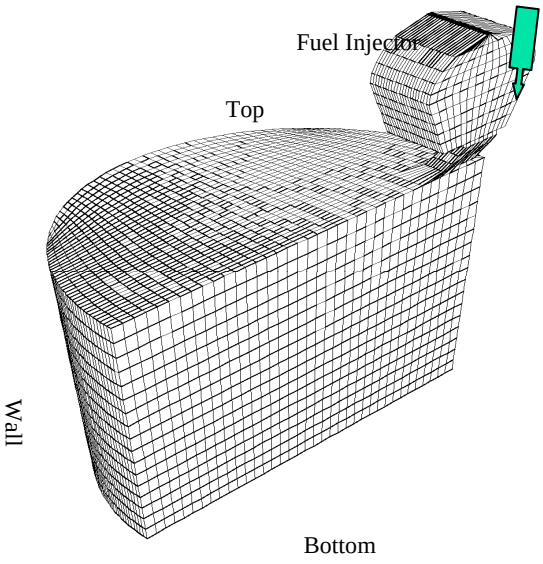

Figure 1: An example of the 3KC1 engine 3-D mesh for calculation purpose (CA=-146º).

The difference between the pressure values of the main and pre-chamber, especially during ignition and early

stages of combustion can be quite significant. Figure 3 shows the calculated maximum and minimum values of cylinder pressure occurring in the combustion chamber at the same moment. The largest difference between the maximum and minimum pressure values can reach as high as 9 bars at around 5 ^{o}CA after TDC, which can demonstrate the magnitudes of the pressure difference between the two chambers for this un-turbocharged engine.

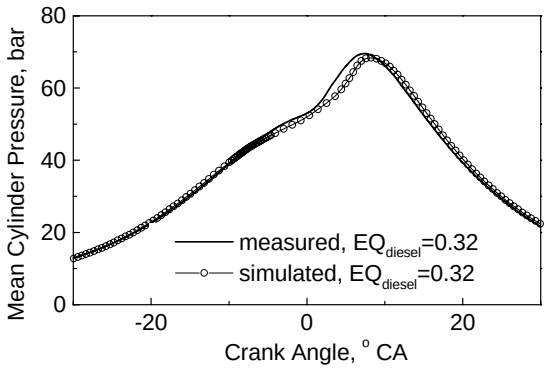

Figure 2: Validation of the model for pure diesel operation.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min with mass flow of diesel: 0.82kg/h

RESULTS

Chamber Surface Temperature Effects on Engine Performance

Compared with the DI diesel engine, the chamber surface temperature for IDI diesel engine has more important influence and associated effects on engine performance and combustion. As can be seen typically in Figure 4, the assumption of uniform and equal temperatures of the main and pre-chamber surfaces can strongly influence key predicted combustion parameters, particularly values of the ignition delay, leading to significant changes in emissions and engine performance, as shown in Figure 5 and Figure 6, respectively.

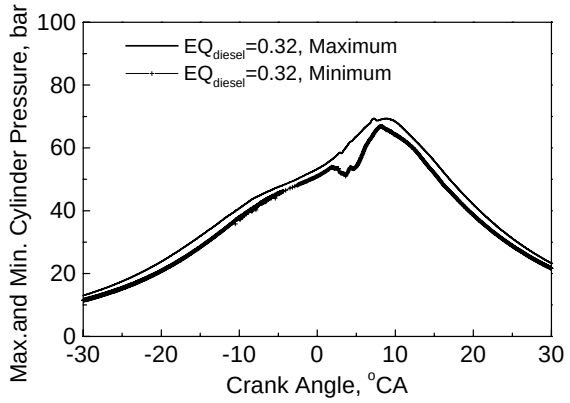

Figure 3: Maximum and minimum cylinder pressures.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C , $T_{coolant}$: 80 °C, n: 1600 rev/min with Mass Flow of diesel:0.823kg/h)

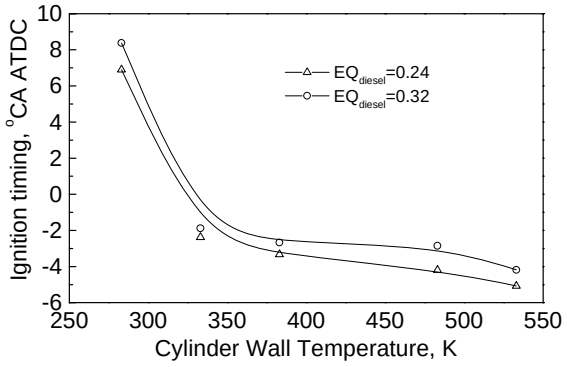

Figure 4: Calculated ignition timing changes with the assumed chamber surface temperature.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

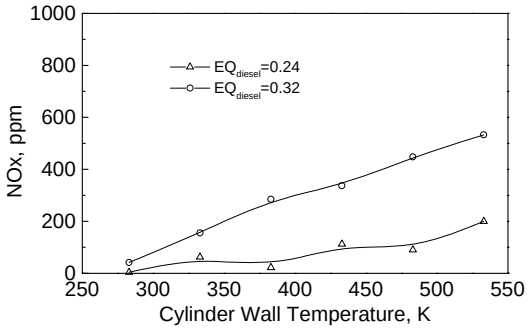

Figure 5: Calculated NOx emissions changes with the assumed chamber surface temperature.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

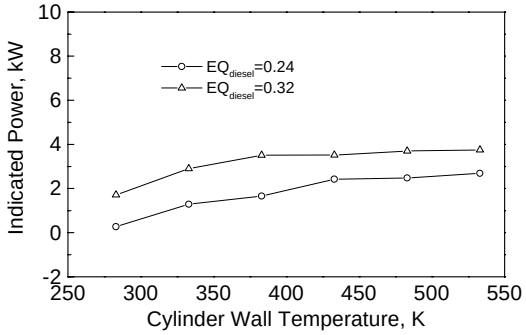

Figure 6: Calculated indicated engine power changes with the assumed chamber surface temperature.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

Nitrogen Addition Effects on Engine Performance

EGR is one of the most effective practical approaches to reduce NOx in diesel engines (Xiao, 2000; Jacobs, 2003; Maiboom, 2008). The bulk and main component of the EGR gas is nitrogen. In order to demonstrate how this approach affects engine performance and effectively reduce NOx emissions simulation was made with nitrogen added in the engine intake from 0 to 20%, by volume. As shown in Figure 7, the indicated power decreases with the addition of nitrogen. A large reduction of nearly 28% in power will incur with the addition of nitrogen reaching

20%. The corresponding changes to NOx emissions can be seen in Figure 8, displaying a dramatic decrease. Therefore, the reduction of NOx via application of EGR is obtained with a penalty in engine power reduction.

Effects of Changes in Spray Cone Angle

It is being increasingly recognized that further improvements to diesel engine performance may be achieved through further improvements and optimization of liquid fuel injection characteristics. Accordingly significant changes in design and operation of fuel delivery systems have been made mainly through empirical type approaches. The employment of predictive approaches to the effects of changes in the system parameters can provide useful guidelines to the development of positive solutions to engine design and operational problems.

The spray cone angle of the injected liquid fuel is the angle for a hollow cone spray during the injection period of the pintle injector as used with an IDI diesel engine. The angle can be varied with changes in the injection pressure, injector geometry, and the prevailing local physical conditions within the combustion chamber. As is shown in Figures 9 and 10, changes in the spray cone angle produce changes in both of indicated power and the NOx emissions. The influence on the latter is particularly very substantial. This would indicate that optimum values need to be employed to ensure proper trade-off between power and emissions.

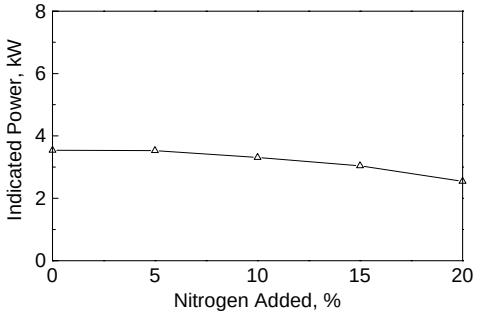

Figure 7: Calculated indicated engine power changes with the added nitrogen.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

Injection timing Effects on Engine Performance

Injection timing is a key important parameter of diesel fuel injection system, affecting greatly both engine performance and emissions. Retarding the injection timing is known effective measure for NOx reduction (Needham, 1990). Simulated results as shown in Figure 11 and Figure 12 demonstrate the extent of changes in the values of the injection timing affecting engine indicated power output and NOx emissions. As an example retardation in the injection timing of 1.0 degree can produce a very dramatic reduction in NOx emissions while to a much lesser extent the indicated power output. Therefore, predictive approaches can be employed to establish a proper trade-off between a reduction in NOx emissions and improvement in power.

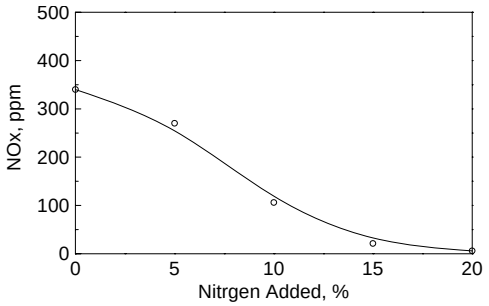

Figure 8: Calculated NOx emissions changes with added nitrogen**.**
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

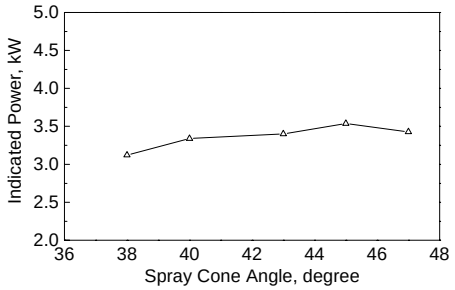

Figure 9: Calculated indicated engine power changes with the spray cone angle.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

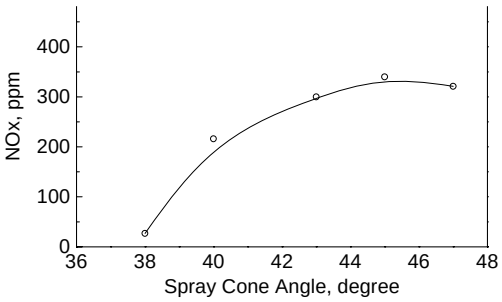

Figure 10: Calculated NOx emissions changes with the spray cone angle.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

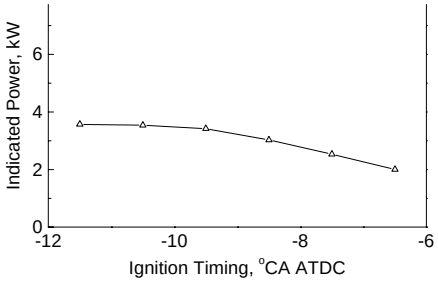

Figure 11: Calculated indicated engine power changes with the injection timing.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

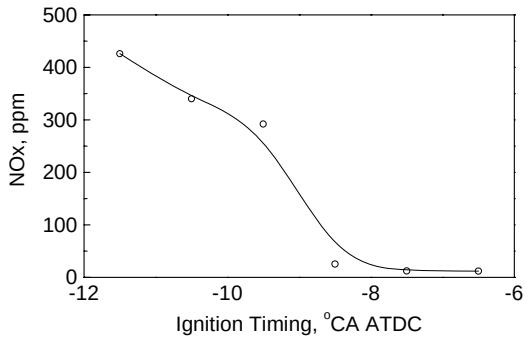

Figure12: Calculated NOx emissions changes with the injection timing.
(P_{in}: 88.30 kPa, T_{in}: 20-26 °C, $T_{coolant}$: 80 °C, n: 1600 rev/min)

Effects of Adding Radicals on Engine Performance

The ignition and combustion processes in diesel engines especially with modern fuel injection systems are critically controlled by the chemical reaction activity of the cylinder charge. Accordingly, it would be highly desirable to enhance this activity artificially for any fuel system which would lead to an improvement in the effective cetane number of the fuel. No successful effective practical approach to achieve this has so far been devised. Moreover, the use of cold EGR dampens drastically such chemical activity. Computational approaches for predicting engine combustion can provide a clear indication of the effectiveness of the chemical sensitization of the charge, which cannot be established normally experimentally.

The addition of some active radical species can accelerate markedly the resulting ignition and oxidation processes (Boyce et al., 1970) as they could probably help to initiate ignition and speed up the chain reactions in fuel combustion process. To explore the effects of adding somehow radicals on engine performance, different concentrations of O, OH, H and HO2 are assumed to be frozen in the intake mixture. Table 1 shows the changes of engine performance and emissions with the addition of these radicals. It can be seen that the extent of merely ten parts per million of radicals can accelerate markedly the resulting ignition and oxidation processes. Therefore, proper account for the extent, composition and role of residual gas cyclically is needed for obtaining good agreement of prediction with experimental values (Liu and Karim, 1996; Wong and Karim, 1999).

Items	Operating Conditions			
	EQ_{diese}=0.32			
	No radicals	Radicals* (ppm)		
		10**	100	1000
Maximum Pressure (bar)	68.4	72.2	72.9	83.4
Indicated Power (kW)	3.54	3.68	3.60	3.51
Ignition Timing (^{o}CA ATDC)	-3.0	-3.1	-3.2	-6.1
NOx (ppm)	340	392	397	509
CO (ppm)	543	355	320	136
CO2 (%)	3.99	4.02	4.05	4.19

Table 1: Comparison of results for different concentrations of some radicals
* OH, H, O, and HO_2
**Values for each

CONCLUSION

Predicted results of the 3-D CFD model developed based on KIVA 3 with a "reduced" detailed chemical kinetics of 291 elementary reaction steps with 79 chemical species for diesel fuel combustion validated well against some corresponding experimental results.

The model was used to predict engine combustion and performance with different varying parameters including chamber surface temperature, nitrogen addition, spray cone angle, and radicals, and it showed the above parameters have significant effects on engine combustion and performance. The model could be used to predicate and optimize the engine performance.

It was evident throughout that the employment of measures to reduce NO_x emissions were associated often with a reduction in engine power.

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