

Numerical Analysis of Diesel Combustion with High EGR and High Boost Pressure using a Multi-Dimensional CFD Code Coupled with Complex Chemistry Analysis

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ABSTRACT

In this study, fuel ignition timing parameters, in-cylinder pressure and heat release rates, and quantities of major exhaust gas emissions from a diesel engine were calculated using multi-dimensional CFD codes coupled with complex chemistry analysis. In addition, a sensitivity analysis of parameters was conducted to identify the major variables affecting these diesel combustion parameters. Firstly, diesel combustion analysis under typical operating conditions was carried out to validate the analytical methods used in the study, and then the effects of intake gas variables (e.g. temperature, and pressure) were investigated in detail in the sensitivity analysis. The results show that the main determinant of ignition timing in the engine is the spatial density of oxygen in the cylinder. This finding indicates that diesel combustion with high EGR and high boost pressure can provide both high thermal efficiency and low emissions.

INTRODUCTION

Multi-dimensional Computational Fluid Dynamics (CFD) simulations of events in engine cylinders and analyses of the detailed chemical kinetics of hydrocarbon fuel combustion have been enabled by improvements in computer performance, the ability to spread calculation costs by parallel processing, and the development of physical models [1]. In contrast, optimization of operating parameters experimentally has become much more difficult and costly because of the complexity of the control systems that have been introduced to meet increasingly stringent emission standards for diesel vehicles. Therefore, use of computer simulations is likely to greatly facilitate and reduce the costs of most, if not all, aspects of engine development.

Recent studies on diesel combustion have shown that long ignition delays promote reductions in PM emissions by lowering the local fuel equivalence ratio, and that reducing the intake oxygen concentration by applying high EGR results in dramatic reductions in NO_x emissions because it

lowers the combustion temperature [2-5]. In this case, fuel ignition timing does not depend on the physical processes involved in the mixing of the fuel vapor and surrounding gases, but on the chemical processes of the auto-ignition reactions, so elementary reactions must be considered to simulate diesel combustion processes. In addition, the spatial distribution of the fuel mixture should be considered in attempts to analyze spray combustion in diesel engines, because it strongly affects the combustion parameters. Accordingly, in this study the combustion processes of a diesel engine were investigated using a commercially available, multi-purpose CFD code coupled with complex chemistry analysis.

This kind of analysis provides a useful way to develop simple real-time combustion models, as demonstrated by various researchers [6-8], to predict diesel combustion characteristics in a short time, since the effects of each parameter can be easily examined numerically by changing the parameters one at a time. In contrast, it is very difficult to change a single parameter experimentally, because almost all of the parameters are correlated with each other. Therefore, sensitivity analysis was conducted, for each parameter, after the accuracy of the models developed in the study had been validated.

EXPERIMENTAL

TEST ENGINE

Results obtained from calculations have to be compared to experimental data to validate their accuracy. The test engine used in this study for validation purposes was an in-line 4 cylinder 2.2L turbocharged diesel engine for passenger cars (see Table 1 for its main specifications).

The following exhaust gases were analyzed, using a HORIBA MEXA-9100 DEGR exhaust gas analyzer, and Non-Dispersive Infra-Red (NDIR) analysis for CO and CO₂, Flame Ionisation Detection (FID) for total hydrocarbons (THC) and chemiluminescence detection for NO and NO_x (NO+NO₂).

Table 1 Engine specifications

Engine type	4-cycle, DOHC, In-line 4, DI
Bore × Stroke	86 mm × 96 mm
Top clearance	0.98 mm
Con-rod length	147.5 mm
Compression ratio	15.8

MODEL FORMULATION

CALCULATION CODE

The CFD code used in this study was a modified form of the commercially available multi-purpose code "STAR-CD version 3.26". The "STAR-CD Complex Chemistry Module" can perform multi-dimensional CFD calculations coupled with complex chemistry analysis.

CALCULATION GRID

The calculation grid used in this study is illustrated in Fig. 1. This grid represents a sector of the cylinder, which is divided by the number of injection holes. Characteristic features of the mesh are that the cell faces are set perpendicular to the fuel spray direction and that the cells the fuel spray passes through are fixed, while the other cells move as the piston moves. This mesh is advantageous for simulating fuel sprays, because parcels are used for the spray calculations, and their positions and velocities are calculated relative to the vertices around them. The number of cells is 5464 at BDC, and 2344 at TDC. The cells are relatively large, but results of preliminary calculations with finer grids showed little difference in calculated in-cylinder pressure and heat release values. So, the coarse mesh was selected to reduce the CPU time.

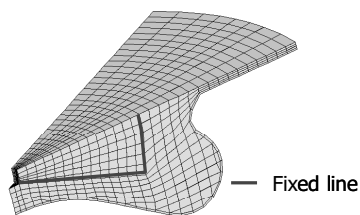


Fig. 1 Sector mesh used in this study

ELEMENTARY REACTION SCHEME

Reduced n-heptane reaction mechanism

An elementary reaction scheme, including each elementary reaction and associated Arrhenius parameters, is required for detailed chemical analysis. However, simulating the reaction mechanism of diesel oil would be extremely difficult, if not impossible, because diesel oil has so many constituents. Instead, N-heptane is often used as a model fuel for detailed chemical analysis of diesel combustion, because the cetane number of n-heptane is very similar to that of diesel oil. A surrogate diesel oil mechanism [9] is also sometimes used in diesel combustion modeling to consider the effect of aromatic

components in diesel oil. However, the n-heptane reaction scheme was used in this study to minimize the CPU time.

Clearly, any model including detailed reaction mechanisms must be able to accurately predict combustion reactions. However, detailed reaction mechanisms must also be simplified in order to complete the analysis within a reasonable CPU time in cases where multi-dimensional CFD analysis is coupled with complex chemistry analysis. Packing isomers and eliminating minor reaction paths can dramatically simplify the reaction mechanism, and Arrhenius parameters can then be modified to trace major reaction paths correctly. In this study, the reduced 'ERC mechanism' reaction mechanism of n-heptane described in [10] and N series reactions described in [11] were integrated. The N series reactions and the Arrhenius parameters applied in this study are summarized in Table 2. The integrated reaction mechanism (the 'Applied mechanism' hereafter) is composed of 33 chemical species and 66 reactions.

Firstly, an analysis based on the ERC mechanism with original Arrhenius parameters was conducted. Tables 3 and 4 show the base simulated conditions and calculation models used in the analyses. The fuel spray breakup model used is the KH-RT break-up model [12], for which major parameters were previously determined in spray visualization experiments in conjunction with parameter optimization [13]. The fuel injection nozzle used in the visualization tests is not the same as the nozzle the test engine is equipped with, but since their specifications are very similar the same parameters were used in the break-up model here. Other calculation models used in the study were standard ones that can be easily selected in STAR-CD and applied to diesel combustion modeling. Calculated results are shown in Fig. 2. When the original ERC mechanism was applied the predicted pressure data (dashed line in the figure) did not show the pressure rise caused by

Table 2 N series reactions applied in this study

Arrhenius' Equation: $k = AT^n \exp(-E/RT)$			
Elementary reaction	A	n	E
$N + NO = N_2 + O$	3.500E+13	0.0	330.0
$N + O_2 = NO + O$	2.650E+12	0.0	6400.0
$N + OH = NO + H$	7.333E+13	0.0	1120.0
$N + CO_2 = NO + CO$	1.900E+11	0.0	3400.0
$N_2 + O = N_2 + O_2$	1.400E+12	0.0	10810.0
$N_2 + O = NO + NO$	2.900E+13	0.0	23150.0
$N_2 + H = N_2 + OH$	4.400E+14	0.0	18880.0
$N_2 + OH = N_2 + HO_2$	2.000E+12	0.0	21060.0
$N_2 + M = N_2 + O + M$	1.300E+11	0.0	59620.0
$H_2/2.00 \ O_2/6.00 \ H_2O/6.00 \ N_2/0.70$			
$NO + HO_2 = NO_2 + OH$	2.110E+12	0.0	-480.0
$NO + O + M = NO_2 + M$	1.060E+20	-1.41	0.0
$H_2/2.00 \ H_2O/6.00 \ CH_4/2.00 \ CO/1.50 \ CO_2/2.00 \ N_2/0.70$			
$NO_2 + O = NO + O_2$	3.900E+12	0.0	-240.0
$NO_2 + H = NO + OH$	1.320E+14	0.0	360.0
$NO_2 + CH_3 = CH_3O + NO$	1.290E+13	0.0	0.0

Table 3 Simulated conditions for the preliminary analysis (these are the 'base conditions' of the sensitivity analysis discussed later)

Engine speed rpm	2000
Intake pressure kPa	100
Fuel injection timing deg. ATDC	0 (TDC)
Fuel quantity mm ³ /st	20
EGR ratio %	19.1
Intake O ₂ concentration vol%	18.5
Intake gas temperature K	344.7

Table 4 Applied calculation models for all of the analyses

Turbulence model	RNG k-epsilon model
Breakup model	KH-RT model sb0=0.61, b1=15.0 ctau=1.0, crt=0.1 We _i =100.0, cb0=17.5
Wall-impingement model	Bai model
Atomization model	Reitz-Diwarkar model
NOx model	Extended Zel'dovich N ₂ O, NO ₂ reactions
Turbulent chemistry interaction model	Kong model [14] C _{mix} =0.01

hot flame reaction. As mentioned above, the parameters in the break-up model were determined in previous work, and the initial temperature, pressure and intake gas constituents were measured in the experiments, so these values were regarded as fixed. The initial composition of the in-cylinder gas was then determined by considering the isenthalpic mixing of the intake gas and residual gas. Therefore, the Arrhenius parameters of some reactions listed in Table 5 were slightly changed to improve the accuracy of the analysis. An in-cylinder pressure curve obtained using the applied mechanism is presented in Fig. 2 (dotted line), in which it can be seen that the numerical code can accurately predict the time course of changes in in-cylinder pressure

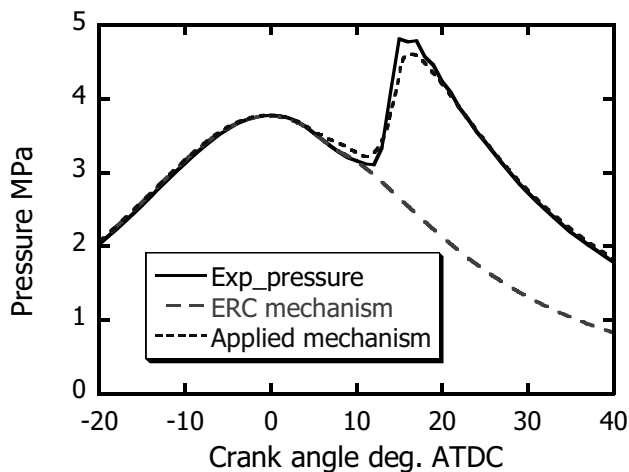


Fig. 2 Comparison of experimental and numerical results of in-cylinder pressure diagrams. (Dashed line, ERC mechanism; dotted line, Applied mechanism)

Table 5 Modifications of Arrhenius parameters used in this study

Arrhenius' Equation: $k = AT^n \exp(-E/RT)$		
Elementary reaction	A	
	ERC [10]	Applied
$C_7H_{16} + HO_2 = C_7H_{15} + 2H_2O_2$	1.65E+13	6.60E+13
$C_7H_{16} + O_2 = C_7H_{15} + 2HO_2$	2.00E+15	8.00E+15
$C_7H_{15} + 2O_2 = C_7H_{15}O_2$	1.56E+12	6.24E+12
$C_7H_{15}O_2 + O_2 = C_7KET12 + OH$	4.50E+14	1.80E+15
$C_7KET12 = C_5H_{11}CO + CH_2O + OH$	9.53E+14	3.81E+15
$C_7H_{15} + 2C_2H_5 = C_2H_5 + C_2H_4 + C_3H_6$	7.05E+14	1.25E+15
$H + O_2 + M = HO_2 + M$	3.60E+17	7.20E+17
$H_2O_2 + M = OH + OH + M$	1.00E+16	2.00E+16
$OH + H_2 = H_2O + H$	1.17E+09	2.34E+09

using optimized parameters, which were used in all the other analysis discussed below, without further modification.

Fig. 3 shows ignition delay times, as a function of temperature, obtained using the mechanism applied in most of the analyses in this study, the ERC scheme, and the detailed reaction mechanism developed by the Lawrence Livermore National Laboratory (LLNL) [15]. The last reaction mechanism in this list (the LLNL mechanism hereafter) includes 560 chemical species and 2537 elementary reactions, so it is claimed to be able to reproduce the reaction process of n-heptane ignition highly accurately. The ignition delay times obtained using the ERC mechanism and the LLNL mechanism were similar, but those obtained with the applied scheme were shorter in the low temperature region (< 1000 K). However, although the ignition delay times obtained using the applied scheme differed from those obtained using the detailed scheme, the predicted in-cylinder pressure diagram for the test conditions agreed well with the experimental data. Thus, since the accuracy of this analysis appeared to be very good, this reaction mechanism and calculation grid were applied in all of the other analyses described below.

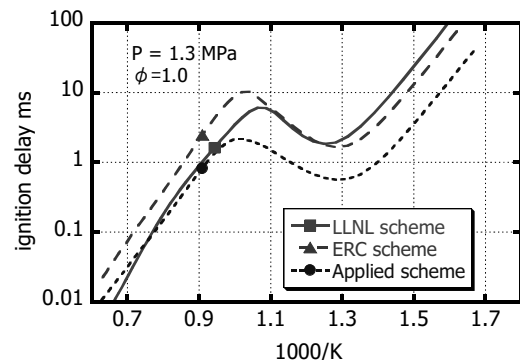


Fig. 3 Ignition delay times as a function of temperature obtained with each of the following reaction schemes: the LLNL mechanism (■), the ERC mechanism (▲) and the Applied mechanism (●).

RESULTS AND DISCUSSION

MODEL VALIDATION

Varied Parameter: Fuel Injection Timing

The first parameter to be varied in assessments of the effects of changing model parameters on in-cylinder pressure and heat release rates was the fuel injection timing. Simulated conditions are shown in Table 6. Intake gas temperatures and components were measured at the intake manifold, and the initial conditions were calculated by considering isenthalpic mixing of the intake gas and residual gas, as previously mentioned. Only CO₂ and H₂O were taken into account as EGR gas components in this study, because the quantities of these species in the in-cylinder gas are very large and strongly affect the combustion characteristics. Fig. 4 shows calculated in-cylinder pressure and heat release rate plots, which clearly agree well with the experimental results, thus the analysis appears to reproduce the effects of variations in fuel injection timing on diesel combustion very well. In addition, Fig. 5 presents a comparison between experimentally and numerically obtained NO_x (NO+NO₂) and NO₂ concentrations. The quantitative prediction of NO₂ is regarded as being very important in diesel combustion analysis, because NO₂ has stronger PM oxidation capacity than oxygen [16]. The predicted NO_x quantity was ca. 20% lower than the measured value, but the calculations adequately captured the experimentally observed trends in NO_x emissions associated with variations in fuel injection timing. In contrast, the predicted quantities of NO₂ were ca. 15 ppm higher than measured values, but the trends in NO₂ emissions, which were independent of the fuel injection timing, could be similarly reproduced. Thus, it can be concluded that trends in NO_x and NO₂ emissions released in diesel combustion could be adequately predicted by the numerical analysis, which was based on the extended Zel'dovich mechanism, NO generation reactions via N₂O, and NO₂ generation reactions.

As described above, the numerical analysis appeared to be able to predict diesel combustion with good accuracy, so calculated in-cylinder gas behavior was assumed to correspond to actual combustion behavior. In-cylinder distributions of gas temperature and NO concentration, obtained by post-processing the calculation results, are illustrated in detail in Fig. 6 to facilitate attempts to explain the effects of varying the injection timing on NO emissions. The images show the ignition timing and the initial

Table 6 Simulated conditions for assessing the effects of varying the fuel injection timing

Engine speed rpm	2000
Intake pressure kPa	100
Fuel injection timing deg. ATDC	-5, -2, 0 (TDC), 2
Fuel quantity mm ³ /st	20
EGR ratio %	30.0
Intake O ₂ concentration vol%	16.2
Intake temperature K	353.15

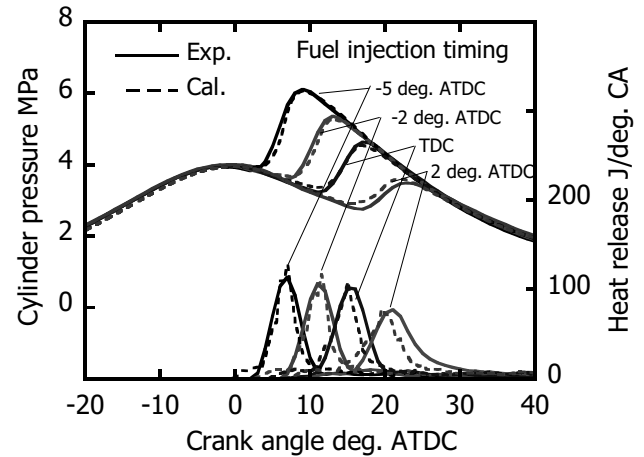


Fig. 4 Comparison of numerically and experimentally acquired in-cylinder pressure and heat release rate curves (varied parameter: fuel injection timing)

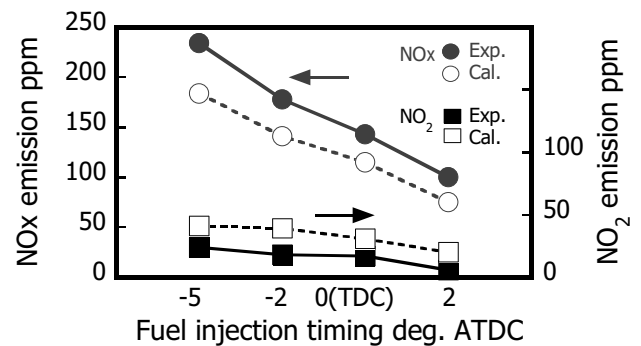


Fig. 5 Comparison of numerically and experimentally acquired NO_x and NO₂ concentrations (varied parameter: fuel injection timing)

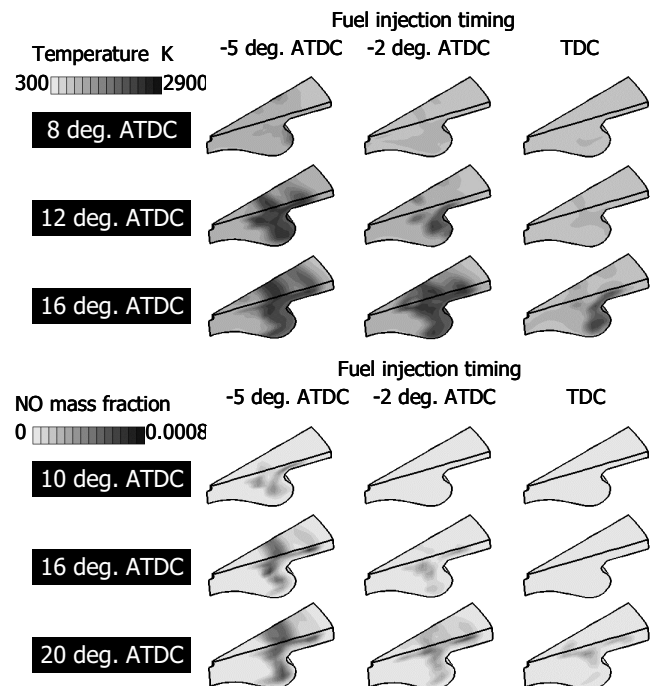


Fig. 6 Calculated in-cylinder distributions of temperature and NO emissions (varied parameter: fuel injection timing)