CI ENGINE MODELING AND EXPERIMENTAL STUDIES FOR LOWER EXHAUST EMISSIONS

[1]Mehmet Zafer GUL, [2]Mustafa YILMAZ, [3]Hasan KÖTEN, [4]Ismail Hakki SAVCI

[1]Marmara University, zgul@marmara.edutr 02163375850
[2]Marmara University, mustafa.yilmaz@marmara.edu.tr, 02163480292
[3]Istanbul Medeniyet University, hasan.koten@medeniyet.edu.tr 02162803202
[4]FORD OTOSAN Company, isavci@ford.com 02165647100

ABSTRACT

In recent years, automotive companies and research centers have utilized different techniques to ensure tightened emission rules. These studies generally are divided into two main categories: in-cylinder and after-treatment applications. In the first stage, harmful exhaust emissions were decreased by optimizing engine parameters. After-treatment applications come into play after exhaust port for irreducible emissions. In the studies, done at Marmara University, three important works examined to get ultra-low emission for a single cylinder diesel engine. In the first study, engine parameters such as compression ratio (CR), intake and exhaust valve timings, mass flow rate were optimized for a range of engine speed. Then for the same engine injection parameters such as start of injection (SOI), injector cone angle, and split injection structures were examined to get optimum parameters for the diesel engine. In CR studies different combustion chambers were tested according to injector cone angles and fuel-wall interaction. In the second study, in addition to the above studies, dual fuel compressed biogas (CBG) and diesel combustion were analyzed under different engine loads both experimentally and computationally. Optimized single fuel diesel cases were compared with CBG + Diesel dual fuel cases which employed port injection for CBG fuel. In dual fuel engine applications, CBG fuel and air mixture is induced from intake port and this air-fuel mixture is ignited by pilot diesel fuel near top dead center (TDC). In dual fuel engine mode, exhaust emissions reduced considerably especially in NOx and particulate matter (PM) because of methane (CH4) rate and optimized engine parameters. The third study is focused on aftertreatment systems to minimize residual exhaust emissions. In this study, computational fluid dynamic (CFD) methodology was developed with conjugate heat transfer, spray, deposit and chemical reaction modeling then emission prediction tool was developed based on the CFD results with deposit prediction mechanism. CFD and deposit results were correlated with image processing tool in flow test bench.

Keywords: CFD, CI engine, emission, optimization, aftertreatment, SCR, NO$_X$

INTRODUCTION

In these investigations, three different works employed to get ultra-low emissions and high performance for a CI engine numerically and experimentally. Multidimensional simulations of the complete engine cycle of diesel engine for single and dual fuel cases are performed and presented here. Moreover, exhaust after-treatment emission modelling methodology are developed for NOx reduction system with experimental and numerical methods.

The intake and compression stroke analyses before the combustion has performed to verify the numerical results with more plausible turbulence model. Then spray and combustion modeling are performed with HCCI strategies in order to achieve clean combustion concept. Following the power stroke simulations emission are also calculated. Furthermore, emission treatment is analyzed in detail for a similar CI engine.

CFD studies for a single cylinder diesel engine were modeled using full engine geometry including intake-exhaust ports and valves. Selected cases were validated by experimental studies. As a result, both in-cylinder optimization studies and after-treatment application study were satisfied EURO6 emission criteria and increased combustion performance with new designed engine concept.

The emissions of the diesel engines consist of various harmful exhaust gases such as carbon monoxide (CO), particulate matter, unburned hydrocarbon (UHC), and nitrogen oxides. Several technologies have been developed to reduce diesel emissions especially NOx reduction systems in last decades [1-7]. The most promising NOx emission reduction technologies are exhaust gas recirculation (EGR) system to reduce peak cylinder temperature that reduces NOx formation caused by combustion and active selective catalyst reduction (SCR) system using reducing agent such as urea-water-solution for exhaust aftertreatment system [8-10].

Recent years many different emission reduction application strategies were developed. One of the challenging approaches is to remove the EGR from the engine, and design a high NOx conversion efficiency SCR with reducing agent system. Thus the comprehensive SCR modeling approach is required

to design compact aftertreatment systems that meet NOx emission legislation level [11-13].

NUMERICAL MODELING

In engine modeling study, optimum operating conditions in a diesel engine fueled with compressed biogas (CBG) and pilot diesel dual fuel were examined. One dimensional (1D), three dimensional (3D) computational fluid dynamics (CFD) code and multi-objective optimization code were employed to investigate the influence of CBG-diesel dual fuel combustion performance and exhaust emissions in a CI engine. In engine studies, 1D engine code and multi-objective optimization code were coupled and evaluated about 15000 cases to define the proper boundary conditions.

3D CFD codes were employed for single diesel fuel and dual fuel (CBG-diesel) cases. Detailed specifications of engine were given in Table 1. In this work, in-cylinder combustion pressure and rate of heat release (ROHR) were evaluated under different operating conditions, engine loads and analyzed the combustion characteristics of the CI engine for single-fuel (diesel) and dual-fuel (CBG-diesel) combustions [14]. Moreover, combustion pressure or indicated mean effective pressure (IMEP), exhaust gas temperature and also Soot, NOx, HC, CO and CO2 exhaust emissions were investigated under different engine operating conditions to investigate the engine performance and exhaust emission characteristics of single-fuel and dual-fuel modes.

Table 1 Engine specifications.

Bore [mm]	76.0
Stroke [mm]	80.5
Displacement volume [cc]	365,25
Number of Cylinders	1
Compression Ratio	17.6
Air intake	Turbo charged

The 3D engine code was used to define the piston movement, intake and exhaust valve lifts. It has been exploited to generate the grid to create the hexahedral cells for the engine model including cylinder head, intake and exhaust ports and piston bowl as shown in Fig 2. The number of cells changed from 500.000 cells in TDC and over 1,700,000 cells in BDC. For the mesh generation hexahedral cells have been accepted since they provided a better accuracy, stability and less computational time compared to tetrahedral cells.
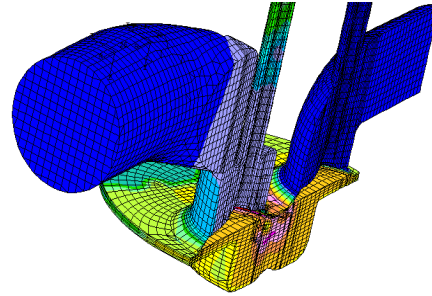

Figure 2 Sectional mesh view for full geometry.

The aftertreatment methodology was developed based on the selective catalyst reduction system after the engine outlet. The developed 3D numerical model accounts for all relevant physical effects. The multi modeling steps were correlated based literature data for each physics such as decomposition process, spray and reducing agent distribution. The influences of flow conditions exhaust system properties and spray parameters on the film formation were evaluated with the developed simple models.
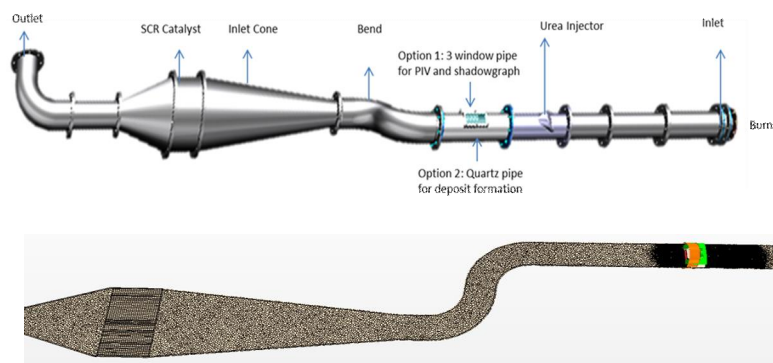

Figure 3. SCR Aftertreatment inline model and computational domain.

The mesh is created using Star-CCM with 2 million elements, including two prism layer around the mixer region to resolve the near wall conditions. The mixer wall and pipe wall are modeled as solid for conjugate heat transfer. Figure 3 shows the computational domain of inline exhaust aftertreatment system

NUMERICAL SIMULATION AND EXPERIMENTAL SETUP

The aim of engine modelling study is to develop engine modelling methodology in CFD. In addition, this methodology was provided proper injection parameters for the homogenous charge compression ignition (HCCI) combustion process for a heavy duty diesel engine. Three conventional type diesel engine cases and four homogenous charge compression ignition (HCCI) type diesel engine cases have been analyzed. The cases were prepared to study the effects of the parameters: start of injection, spray angle and spray profile. Two kinds of injection strategies, conventional diesel direct injection and two stage injection (split injection), were examined. The results confirmed that the split injection strategy is more effective in reducing NOx emissions than the direct injection (DI) diesel engine while maintaining high thermal efficiency. Also, it has been found that, the split injection strategy with narrow cone angle fuel injection has the potential for reducing CO emissions by optimizing both injection timings and piston bowl geometry.

Different injection parameters and their combinations were examined to understand how they effect on combustion process. Detailed investigations of cold flow, spray and combustion phenomenon for a heavy-duty CI engine were performed by Yilmaz [15,16]. In these cases, start of injection (SOI), spray angle and spray profile were changing. Table.2 and Table.3 shows the distinctive marks of the test engine and cases that are compared with each other.

Table 2 Some properties of the test engine

Engine parameters	Value
Type	1 Cylinder
Bore × Stroke	104×145 mm
Connecting rod length	231.2 mm
Compression ratio	19.75:1
Max. Lift (exhaust)	10,4 mm
Max. Lift (intake)	9,9 mm
Operating speed	1000 rpm

Three conventional cases which have cone angle of 149° CA and compression ratio of 19.75:1 are simulated in different SOI conditions. The proper case of these three conventional cases which has minimum NOx and CO is selected. Moreover, HCCI cases which have the same compression ratio and SOI of 120° CA TDC with two different cone angles

of 80° and 60° CA were performed. Similarly, last two HCCI cases were performed in different compression ratios of 16.27:1 and same cone angles condition. In similar conditions cases were compared each other.

Table 3 Case studies

Type	Case #	Cone angle	SOI CA	Injection profile		Compression ratio
Conventional diesel	0		-20			
	1	149°	-25	single		19.75
	2		-15			
Narrow angle	3	80°	-120 -12 +6	Pre Main Post	30% 65% 5%	19.75
	4	60°	-120 -12 +6	Pre Main Post	30% 65% 5%	19.75
	5	80°	-120 -12 +6	Pre Main Post	30% 65% 5%	16.27
	6	60°	-120 -12 +6	Pre Main Post	30% 65% 5%	16.27

The conventional type diesel engine processes are shown in the first three cases. Other cases denote the Partially Premixed Compression Ignition (PPCI) type diesel engine. Effect of mass flow rate on the emissions and total heat release were examined in the first three cases. For both three cases total injected mass per cycle is same, but SOI and end of injection (EOI) are vary, so the mass flow rates are different.

The lower diesel fuel consumption (dodecane-2.14 kg/h) caused the reduction on the combustion performance as shown in figure 4 (a). When it came to the 60% load, shown in Fig. 4 (a), the diesel combustion showed slightly higher peak combustion pressure (Pmax = 8.4 MPa) and peak heat release compared to CBG-diesel case (Pmax = 8.3 MPa). Simultaneously, a greater indicated mean effective pressure (IMEP) was obtained for single fuel diesel injected fuel mass reached 5.3 kg/h. Figure 4(b) shows effects of dual fuels on the combustion characteristics with different engine loads.
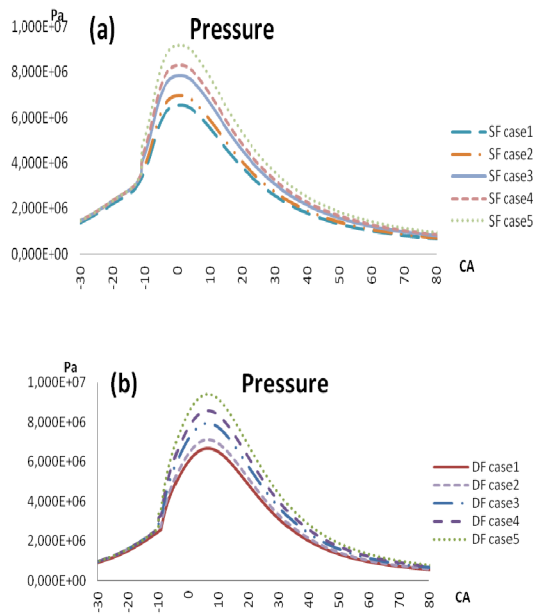
Figure 4 Combustion characteristics at different engine load. (a) Single fuel (dodecane) cases. (b) Dual fuel (CBG+dodecane) cases.

The concentrations of NOx emissions for the engine operated with single and dual-fuel combustion modes were shown in Fig. 5. In Fig. 5, when the engine load increased, NOx concentrations of all test cases increased steeply. Significantly lower NOx emissions were emitted within the dual-fuel operations compared to the single mode at all conducted test ranges. In Fig. 5, single fuel diesel combustion cases resulted in higher NOx emissions at all engine loads compared to dual fuel cases. The reason behind this trend could be explained by the faster injection and early ignition characteristics of diesel which are visible in previous outcomes of combustion characteristics.
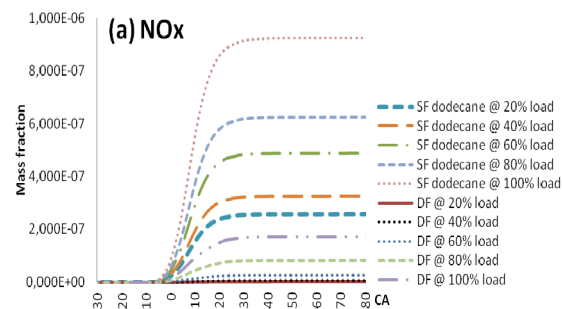

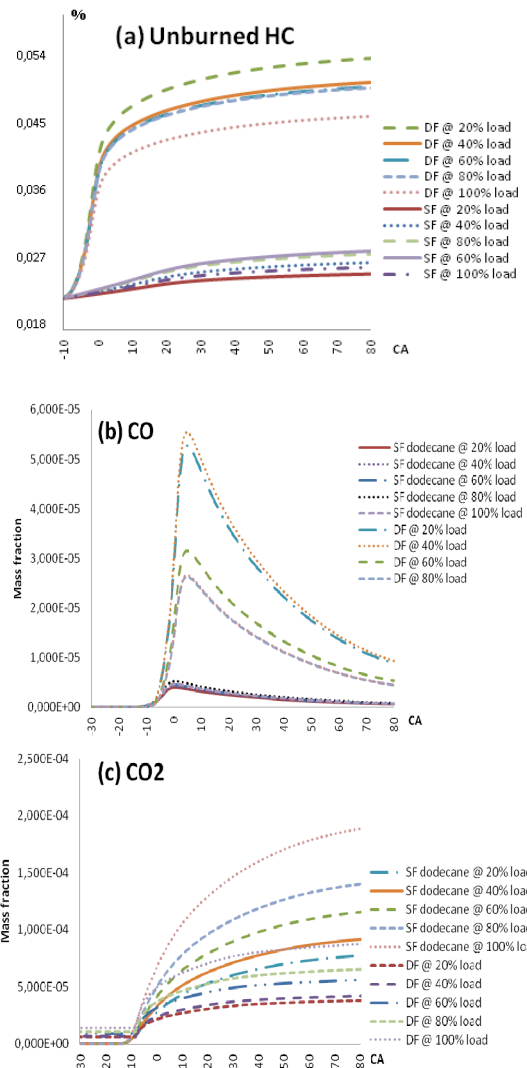**Figure 5.** NOx for single and dual fuel cases versus CA.

Figure 6 Exhaust emissions for single and dual fuel cases with different engine loads.

In fig. 6 (a), (b) and (c) for single and dual fuel cases at various engine loads, CO_2, HC and CO concentrations were shown. In dual fuel cases, gaseous fuel induced during the intake stroke, this air fuel mixture decreases the charge temperature and affects combustion performance and exhaust emissions. Ignition delay takes longer time in dual fuel cases because of decrease charge temperature and lower cetane number. For this reason, in dual fuel combustion cases concentrations of HC and CO emissions bigger than single fuel cases. In figure 6 (a) HC emissions decreased by increase of engine loads due to the increase of combustion temperature. Similarly, in figure 6 (b) CO concentrations decreased due to the increase of temperature inside the combustion chamber by engine loads. CO_2 content of CBG is ingested during the intake process clearly seen in figure 6 (c). For single fuel cases CO_2 emissions are higher than dual fuel cases when compared to CO_2 content of CBG-dodecane dual fuel cases. Carbon content of single fuel cases are

relatively higher than dual fuel cases, resulting significantly increase in CO_2 emissions. As shown in these figures, the concentrations of CO_2 emissions for dual fuel were obviously under those regarding single diesel combustion modes. Moreover, higher cetane number of diesel and the faster injection timing shortened the ignition delay and this reduction is related to a decrease in fuel-rich zone throughout the combustion process [3]. When single and dual-fuel combustions were compared, the concentrations of HC and CO emissions for the single-fuel mode were considerably lower than dual-fuel mode under all test conditions. CBG-air mixture needs to reach the specific temperature value to continue the flame propagation in the combustion region. CO emissions for single fuel combustion emitted somewhat lower and roughly constant amounts of soot in comparison to dual fuel combustion.

The last emission prediction work is aftertreatment modeling [17]. The aim of this work is to develop comprehensive approach to predict exhaust emission for selective catalyst reduction. The emission prediction is assessed by 1D modeling tools. The complex physics are modeling by 3D simulations of exhaust gas aftertreatment systems.

The CFD software calculates the conjugate heat transfer, flow field, spray modeling, species distribution and deposit modeling in the SCR systems. These results are calibrated by using the experimental data coming from the PIV, shadowgraph measurement in flow test bench and dyno test bench. Figure 7 shows the test bench for the exhaust aftertreatment modeling setup. PIV and shadowgraph was occurred to get velocity distribution and particle sizes.

The measurements are performed under a wide range of transient and steady state operating conditions. For this work flow test bench is built with compressor, burner and automation system.
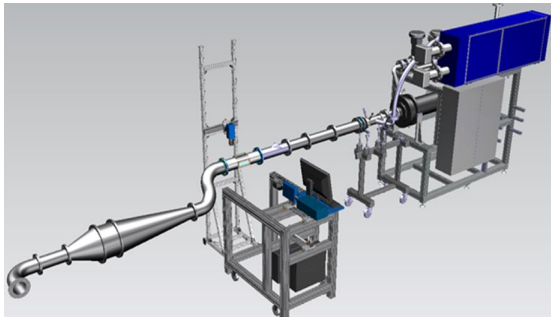

Figure 7. Schematic of Exhaust System Layout with Emission

Since deposit has complex phenomenological physics for 1D emission prediction tool is required whether the design meet the emission legislation target. This emission prediction tool should be fast and accurate method with 3D simulation and deposit effect on the SCR system. Before freezing the design of SCR system, emission level of design should be predictable whether further design optimizations or advanced SCR technologies are required. 1D emission tool can predict to different SCR catalyst sizing, chemical kinetic effect and different aftertreatment system layout on emission level.

RESULTS AND DISCUSSION

Figure 8 shows the example of the combustion characteristics of conventional diesel combustion attained by single injection [16]. In the case of conventional diesel, combustion starts by injection at 15°, 20°, 25° bTDC, as shown in Fig. 8. In these first three cases, the ignition delay was very short and ignition had begun during injection event. This led to significant in homogeneity during combustion. Corollary, high emission results such as NOx and soot could be expected as seen in Fig. 10. NOx emission decreases for conventional diesel engines when the distance between the start of the injection and TDC is larger. Because of the high temperature and heat release, NOx emission results higher and soot emission results lower than the other cases.
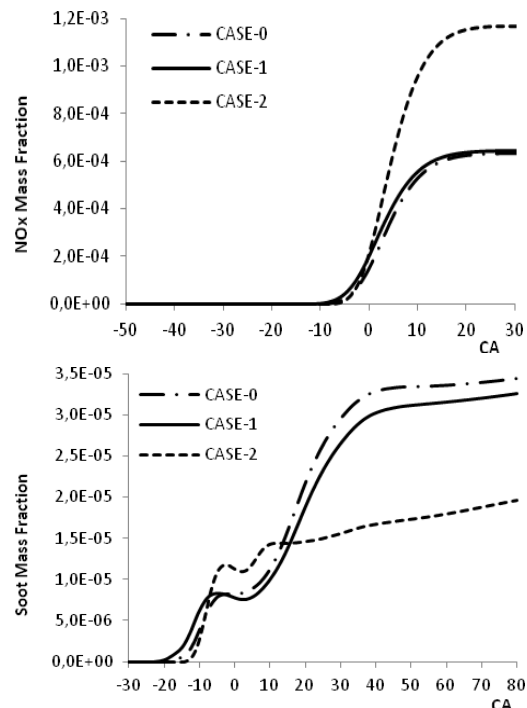

Figure 8 Injection rates and results for conventional cases.

NOx and soot emissions showed a strong dependence on the injection timing at a constant equivalence ratio. The peaks of the NOx emissions occurred between -10° and 20° which were slightly

advanced of the injection timing as typical of the operating conditions of a conventional diesel engine as shown in Figure 8.

Figure 9 shows the example of the combustion characteristics of PPCI diesel combustion attained by split injection. In this split injection strategy pre, main and post injections have 35%, 60%, 5% of fuel per stroke respectively with 80° and 60° narrow angle.
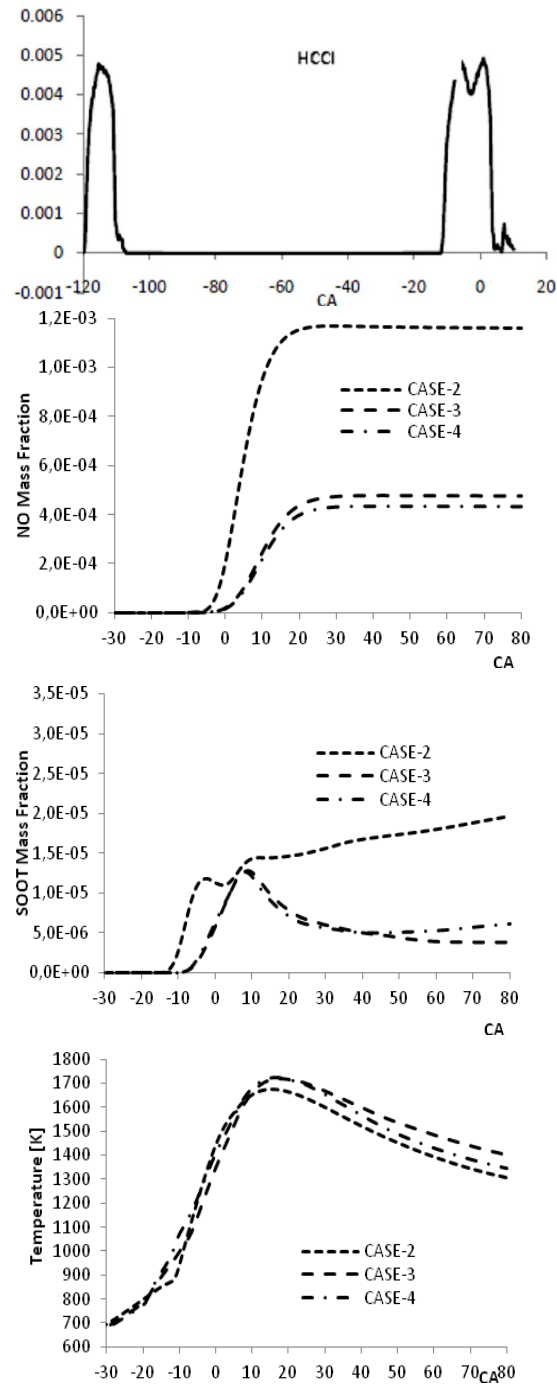
Figure 9 Comparison of the results for different the spray angles

In these cases, the ignition delay was very long and ignition had begun before main injection event close to TDC about 23° bTDC. This led to significant homogeneity during combustion. Corollary, low emission results such as NOx and soot could be expected.
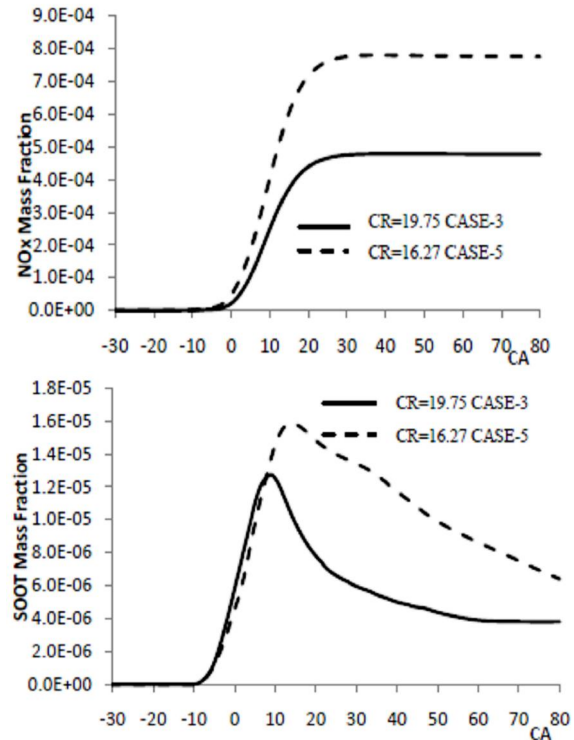
Figure 10 Comparison of the best PPCI cases according to emission performance for different compression ratio.

The results for PPCI cases shows that, case3 which is prepared with using 80° cone gives better emission performance for both soot and NOx emissions relative to case4 with 60° cone angle. PPCI cases were compared to obtain optimum case for NOx and soot emissions. Fig. 8 shows the results for these cases.

The injection profile has a consequential effect on the emissions as seen in the Fig. 11. The soot emission results show that partially-premixed type injection model reduces this emission. However, NOx emission fraction for case2 is much more than the other cases due to the single type injection of fuel and start of the injection. The pre-injection (%30 of total fuel per stroke) makes the average temperature in-cylinder higher than the other cases as seen in the Fig. 11. Locally high temperatures (~2700K) are formed especially at the regions close to the injection point. Same results occur in the case3, case4, case5, case6, which includes %30 pre-injection fuel mass. Case3 gives the best results for soot and NOx emissions. Fig. 11 shows that there is an improvement on emissions with narrow cone angles

and split injection strategy. The soot and NOx emissions decrease for PPCI cases which includes narrow spray angles although there is high in-cylinder temperature relative to conventional cases. PPCI results show that case3 in which the injector has 80° cone angle results in lowest emissions.

On engine geometry, compression ratio was reduced from 19.75:1 to 16.27:1 by decreasing maximum radius of the bowl and increasing the depth of the bowl to prevent the immoderately advanced ignition

of the pre-mixture formed by early injection Table 3. Because of its effects on in-cylinder temperature and pressure during the compression phase, the engine compression ratio has an influence on the auto-ignition phase of the combustion: a reduction prolongs the air/fuel mixing process before combustion. Different works, performed on experimental single cylinder engines showed this significant advantage [16].
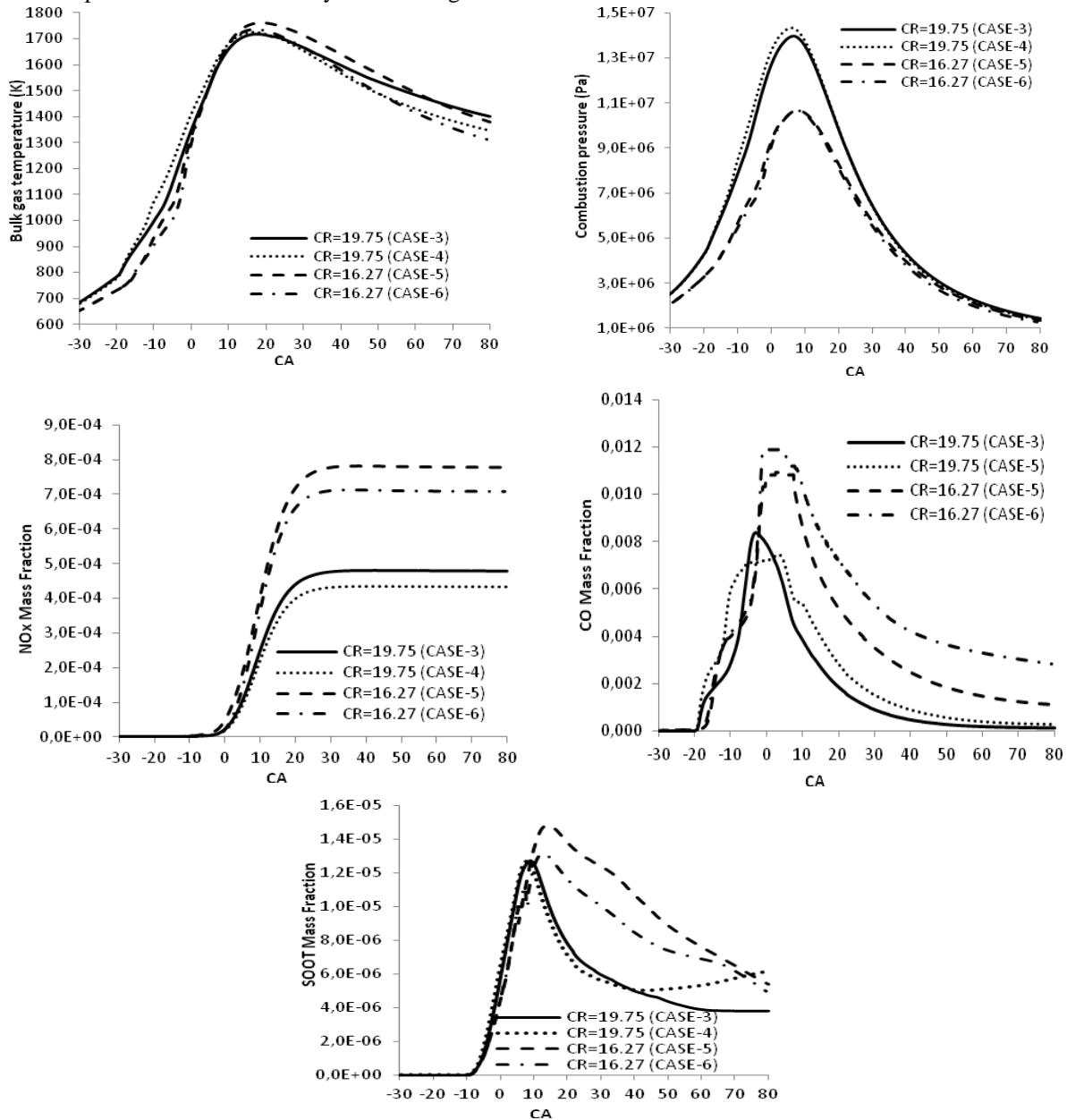
Figure 11 Effects of the compression ratio

According to soot emission results show to reduce the compression ratio increases emission values. Both of NOx and soot emission fractions for case5 is much more than for case3 due to compression ratio value. Reducing compression ratio should be made

the average temperature and pressure in-cylinder higher than the other cases but not. Because of the high temperature and heat release, NOx and soot emission results are higher than other cases. Same results occur in the case6, which includes less

compression ratio value. Case3 gives the best results for soot and NOx emissions. Case3&5 which use 120 degree CA bTDC as a start of the injection time, has better emission values than the other two cases.

The results are shown in Fig.11 show that although there is a rise on the mass fraction of the soot, the NOx value for case4 which uses a narrow spray angle of with 60°, is better than case3. The peaks of the temperature occurred unexpectedly at cases have reduced compression ratio (16.27). Therefore, these two cases have indicated that the high temperature reaction (HTR) occurs at around 1000÷1100 K. The calculated peak of the bulk gas temperature for reduced compression ratio as shown in Fig.13 was about 1800 K such as conventional diesel combustion, clearly lower than NOx formation temperature but higher than other PPCI cases.

As the compression ratio reduced, the peaks of heat release rate of HTR rapidly increased and the initiating timings of the reaction were also retarded. In these cases, the ignition delay was very long and ignition had begun before main injection event close to TDC about 20°-25° bTDC. This led to significant homogeneity and better combustion control during combustion. However, higher emissions such as NOx and CO could be unexpected. Only soot emissions consequently slightly decreased and kept reduction

trend. Furthermore, it could be said that fuel is burned effectively with respect to other cases (Fig.11) especially for case4 has reduced compression ratio (case6).

The efficient design of selective catalyst reduction system is required to NOx reduction mechanism. This system design is crucial for emission legislation. In this study, comprehensive modeling approach has been developed to simulate active SCR system based on inline exhaust aftertreatment system from Flow Test Bench. By This method we can understand whether the design/design changes effect on emission. [10-13, 17, 18]

Three dimensional (3D) simulation of inline exhaust aftreatment system with spray injection of UWS, evaporation and thermal decomposition processes have been presented results in the present chapter using Star-CCM [17]. The deposit prediction of the CFD result was correlated with flow lab image processing. Then the deposit mass increased and ammonia mass flow rate are reduced based on the flow lab test results. The correlated values of ammonia are passes to emission prediction model. [18]
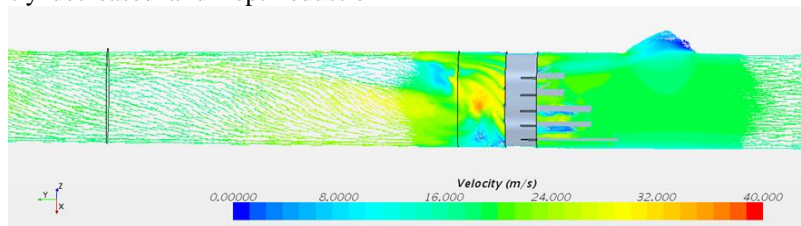

Figure 12. Velocity vector at the cone k-epsilon

The velocity fields are investigated in details. The turbulence model of the RSM predict in good agreement of the flow recirculation at the upstream

of the catalyst. k-ε turbulence model cannot predict the swirl region upstream of the mixer in Figure 12.
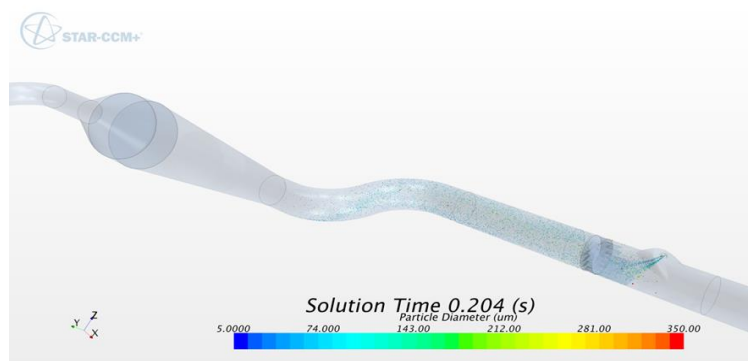

Figure 13. Droplet Distribution across the system at 0.1325 **s**

The mixers are installed at the downstream of the injector of the inner pipe. They are enhanced droplet

evaporation, breakup and distribution of the spray. [19] The mixer has significant effect on the break-

up process. Figure 13.shows the application of mixer. [20]

Emission results of the inline exhaust aftertreatment system shows high temperature operating point NOx conversions are %98.
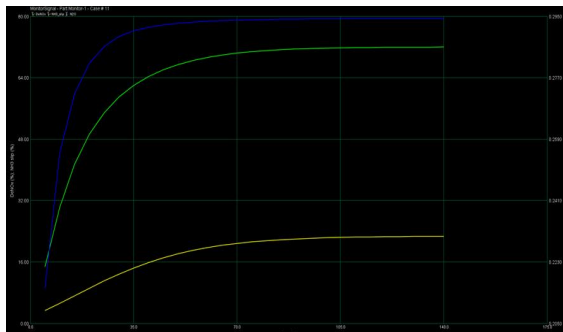

Figure 14. WHSC point for NH3 distribution from CFD

Figure 14.shows emission result of the inline exhaust aftertreatment system. For high temperature operating point NOx conversions are %98.

CONCLUSION

In this work, three main studies; effects of engine parameters on the diesel engine performance, effects of dual fuels on the diesel engine performance and aftertreatment system investigations were studied and presented. Various configurations of compression ratio, injection timing, cone angle and bowl geometry are compared to get the best performance of the engine. Obtained CFD results are found qualitatively in agreement with the previous experimental and computational studies in the literature.

In the present study new combustion model (ECFM-3Z) is used successfully. Moreover, on an engine configuration with compression, spray injection and combustion in a DI Diesel engine are satisfactorily modeled. Effect of combustion chamber design and injection parameters for single and dual fuels in a DI diesel engine are investigated and presented. Simulations how the injection parameters affect emissions, show that the emission results under some PPCI circumstances may be highly affected by a relatively small change of injection rates. Multicomponent UWS injection modelling and multi reaction modeling as thermolysis and hydrolysis have been implemented into inline exhaust aftertreatment system and validated with literature work and flow test bench capabilities as pressure, temperature NOx and FTIR information. The PIV gives reasonable result to correlate this complex SCR system.

The developed numerical simulations for droplet and species show the dependency of the SCR system to the injection characteristics and flow field parameters. The good agreement is shown in terms of injection and flow field between numerical model and flow test bench.

The simulation of active SCR system has been performed in spray-wall interaction framework as well. The multi component Bai impingement model has been adopted into numerical simulation to predict deposit location but mass of deposit cannot predict well.

These comprehensive 1D emission models are used to predict emission level in WHSC cycle and compared the dyno test results. These results are comparable well. Considering the results of this work, following conclusions can be drawn:

The present work revealed that Reynolds stress turbulence model is sufficient to model. PIV measurement and RSM simulations may be employed to directly validate turbulent exhaust flow field and spray simulation.

The heat transfer correlation work of inline exhaust aftertreatment system shows conjugate heat transfer is required.

In addition to serving their primary purpose of enhancing mixing between exhaust gas and spray, mixers are quite effective in reducing deposits. Heat transfer via spraying onto a mixer's hot surfaces results in enhanced boiling and convective heat flux. Mixers with large surface area are promising in enhancing particularly conjugate heat transfer despite the fact that mixers often reduce spray particle transport length. System design has a significant impact on the system performance and formation of the deposit.

The pipe surface temperature is a critical factor due to the deposits that form on the inner pipe walls of the system. Below a certain critical temperature, wall wetting and ensuing deposit formation are built.

1D emission prediction models with species, velocity and temperature data from 3D CFD at the SCR inlet and deposit mapping from image processing tool shows the good validation according to engine dyno data.

NOMENCLATURE

1D   : One-Dimensional
3D   : Three-Dimensional
aBDC : After bottom dead center
aTDC : After top dead center
BDC   : Bottom dead center
Bsfc : Brake specific fuel consumption (g/kWh)
CA   : Crank Angle
CAD   : Crank angle degree

CFD   :Computational Fluid Dynamics
CI   : Compression ignition
CO   : Carbon monoxide
CO   :Carbon Monoxide
EC   :European Commission
EGR   :Exhaust Gas Recirculation
NOx   :Nitrogen Oxides
PM   :Particulate Matter
SCR   :Selective Catalytic Reduction

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