Modified Selective Non-Catalytic Reduction System to Reduce NOx Gas Emission in Biodiesel Powered Engines

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ABSTRACT

Biodiesel is considered as one of the attractive alternatives to fossil diesel fuel. Although biodiesels reduces most of the harmful gas emissions, they normally releases higher NOx emissions compared to fossil diesel. The Selective Catalytic Reduction (SCR) is a well-known technique used in the OEM industry to mitigate NOx emission. However, this technique may not be suitable for application in low power density engines due to back pressure and clogging issues. On the other hand, Selective Non-Catalytic Reduction (SNCR) is used in relatively large combustion operations ie. boilers and incinerators. The main disadvantage of SNCR technique is the high temperature window for diesel engine exhaust temperature. This study introduces a new design concept, which is a combination of SCR and SNCR systems, for low power density diesel engines. The developed after-treatment system composed of two main parts, injection-expansion pipe and swirl chamber. The working principle is providing maximum mixing of the injected fluid and exhaust gas in the expansion chamber, then creating a maximum turbulence in the swirl chamber. In this regard, NOx emission can be reduced at relatively lower exhaust temperatures without using any catalyst. The CFD models of three design candidates were examined in terms of velocity magnitudes, turbulence intensity and particle residence time to select the optimum physical dimensions. The selected design was manufactured and installed to exhaust system of a 1.3 litre diesel engine. Two fluids distilled water and urea-water solution were injected separately at the same flow rate of 375 ml/min. Exhaust gas emissions of fossil diesel, sheep fat biodiesel – waste cooking oil biodiesel blend and chicken fat – cottonseed biodiesel blend were tested. No significant changes in CO_2 and HC emissions were observed. However, it was found that distilled water injection reduced CO and NO emissions by about 10% and 6% for fossil diesel; and by about 9% and 7% for biodiesels operation respectively. The urea-water injection led to reductions in CO and NO emissions by about 60% and 13% for fossil diesel; and by about 45% and 15% for biodiesels respectively.

KEYWORDS

Biodiesel, after-treatment, NO emission, CI Engine, NOx control, combustion, exhaust emissions

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INTRODUCTION

The biodiesels are viable alternatives to replace fossil diesel [1, 2]. They are renewable, biodegradable, carbon neutral, energy efficient and can be used in compression ignition (CI) engines without any modification [2]. In addition, most of the exhaust gas emissions such as CO, CO_2, HC and smoke intensity are reduce with biodiesels compared to fossil diesel [3,4]. However, NOx emissions of in biodiesels operation are reported to be comparable or slightly higher relative to diesel operation [5]. According to Thangaraja et al [6], 85% of the published literature reported that NOx emission was increased for biodiesel powered CI engines, while only about 10% of the literature reported no change in NOx gas emission compared to diesel. Interestingly, only 5% of the literature found NOx reduced with biodiesels. The reason underlies on the increased combustion temperature as a result of the higher oxygen content of biofuels which provides improved combustion. Therefore, it is decided to cope with the NOx penalty at the exhaust system by a help of after treatment system.

In this regard, the latest technology found is ammonia injection after the combustion process i.e. at the exhaust system [7]. One application of this technique is Selective Non-Catalytic Reduction (SNCR) which generally used in relatively large engines, furnaces, incineration or boilers. SNCR system injects diesel exhaust fluid (DEF – ammonia) directly into the exhaust system without any catalyst. Another application is Selective Catalytic Reduction (SCR) which also involves catalytic to upgrade the NOx reduction yield. Because of the cost of catalyst, it is mainly used in relatively small size applications such as the automotive sector.

The SCR was first found in the 1970s and commercialised in Japan around 1957 [8]. The operational temperature of the system is reported above 350°C [9]. Literature reported NOx reductions of up to 90% with the application of SCR after treatment system [10]. However, these extreme NOx mitigations came up with well-developed designs providing controlled NH_3 to NOx ratio and uniform velocity through the catalyst [10]. Even though SCR is a very effective technique, there are some drawbacks due to the presence of a catalyst such as erosion (because of dust or ammonium bisulphate), limited lifetime, mass transfer, expense and possibility of catalytic disintegration which cause an additional source of pollutant [8,11,12]. These problems can be avoided with SNCR system which is free of catalyst. However, SNCR systems have the operating temperature between 875°C and 1050°C, thus they are mainly used in large stationary units like boilers, furnaces and incineration [13]. This is mainly due to the lower reaction rate between ammonia and NOx below 800°C; hence the injected ammonia does not properly react with the exhaust gas. On the other hand, above 1200°C temperature, ammonia oxidises and starts forming NO which increases the emissions [14]. Mansha et al, [15] proved these conditions with a numerical study. They studied NOx reduction by utilising SNCR technique and predicted up to 96% reduction of thermal NOx under the conditions of; molar ratio of 1; the temperature at 800°C and residence time 2.5 seconds [15]. The major barrier of SNCR technique for diesel engine application is the high-temperature window (i.e. operation range between 875°C and 1050°C) [16]. To avoid this issue, studies have tried various solutions such as implementing an extra mixing chamber to enhance the turbulence [17], double compression expansion engines to increase the exhaust temperature [16], various additives and/or injection agents [18] and injecting aqueous urea solution directly into the combustion chamber after the fuel injection [19]. For example, Thiyagarajan *et al.,* [17] studied SNCR technique with an extra mixing chamber on a single cylinder CI engine on diesel operation. They have tested four different injection agents which were anhydrous ammonia, succinic acid, diethylamine and monoethanolamine at 1 kg/h flow rate. They reported maximum reductions of 10% and 15% for NO and CO_2 emissions with monoethanolamine injection at full load. Muric *et al.,* [16] used double compression expansion engine and reported 55% reduction on NOx emission at 1200 rpm and 1200 K temperature. However, the same study also provided 10-22% NOx reduction at 1000 K exhaust temperature. In another study, Krahl *et al.,* [18] tested 1,2,3-tris-(diethylaminomethoxy)propane, 1,2-Bis-(diethylaminomethoxy)-3-ter/-butoxy propane and 2,2-dimethyl-(4-diethylaminomethoxy)-1,3-dioxolane additives with SNCR and obtained 22% NOx reduction for diesel and 47% NOx reduction for biodiesel. Yang *et al.,* [19] used a separate injector to inject urea-water solution directly into the combustion chamber during the power stroke, they reported NOx reduction up to about 53%.

Based on the literature review, three parameters such as mixing (turbulence), exhaust temperature and residence time are found critical for SNCR efficiency. Therefore, the aim of this study is to design and test a novel SNCR after treatment system for CI engine application with a special emphasis on NOx reduction. By this means, NOx penalty of biodiesels will be lowered and catalytic problems of SCR will be avoided. The new design is composed of two parts which are expansion and swirl chambers. Enhanced turbulence intensity and residence time are desired to improve NOx reduction of biodiesel as well as diesel. The CFD analysis of design options is carried out to select the best design geometry in terms of turbulence intensity and injected particle residence time. Then, the selected design was manufactured and implemented on the test rig for experimental analysis. The objectives of the current study are: (i) to select after treatment system components which will maximise the turbulence and residence time, (ii) to select an optimum concept and dimensions through CFD modelling and, (iii) to implement and test the after treatment system on the compression ignition (CI) engine fuelled with biodiesels. The biodiesels used in this study was mixture of waste cooking oil biodiesel and sheep fat biodiesel at 50/50 volume fraction (W50A50); and cottonseed oil biodiesel and chicken fat biodiesel mixture at 50/50 volume fraction (CO50CH50). A multi-cylinder indirect injection engine was used in the study.

METHODOLOGY

NOx decomposition reaction mechanism

Ammonia is a well-known chemical that reacts with nitrogen oxides and forms nitrogen and water which are not harmful. However, ammonia itself is a dangerous chemical. Therefore, it is commonly stored and transferred in the form of urea $CO(NH_2)_2$. Typically, urea-water solution is used for injection through after treatment systems. Then the urea decomposes into ammonia in the presence of water as shown in equation 1 [20]. This process takes place above 350°C with a residence time minimum of 0.1 s [20].

$$CO(NH_2)_2 + H_2O \rightarrow 2NH_3 + CO_2 \tag{1}$$

The three possible reaction mechanisms of NOx reduction in the presence of ammonia are illustrated in equations 2, 3 and 4 [20–23].

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \tag{2}$$

$$4NH_3 + 2NO_2 + O_2 \rightarrow 3N_2 + 6H_2O \tag{3}$$

$$2NH_3 + NO_2 + NO \rightarrow 2N_2 + 3H_2O \tag{4}$$

The required amount of urea for an application can be calculated through the introduced equations. In this research, it was assumed that all NO will be converted through equation 2 and all NO_2 will be converted through equation 3. The equation 4 was not considered as it also requires the same molar ratio with the equations 2 and 3 (2 moles of NH_3 is required to convert 1 mole of NO_2 and 1 mole of NO). Ultimately, 1 mole of NH_3 is needed to decompose 1 mole of NO; and 2 moles of NH_3 is required for decomposing 1 mole of NO_2.

Injection flow rate

Although the rated speed of the engine was 1500 rpm, the after-treatment system was tested at 2000 rpm and 80% engine load (11.2 kW). This was simply because to meet the exhaust temperature limitations of the low power density engine. The exhaust temperature was around 380 °C at the mentioned condition. Exhaust heat wrap also applied to retain the heat at the exhaust pipe.

The NO and NO_2 emissions for the biodiesel were previously measured as 1.408 g and 0.840 g through Horiba gas analyser. Considering these emissions, approximately 1.4 g of ammonia per second is required to be injected at the exhaust pipe. This corresponds to around 2.2 g of urea. The commercial Diesel Exhaust Fluids (DEF - AdBlue) are generally composed of %32.5 urea solution in deionised water. As a commercially available DEF was used in this study, the flow rate of the %32.5 urea solution in deionised water was calculated as 308 ml/min.

Design concepts

Three exhaust after treatment geometries were developed and modelled in ANSYS FLUENT software version 17.1 to figure out the best geometry Figure 1. The idea of the system was to inject the commercially available urea-water solution (AdBlue) but avoiding the catalytic; as the use of catalytic cannot be suitable for low power density engines which cannot cope with high back pressures. In this regard, it was planned to increase both turbulence intensity and particle residence time of the catalytic free system.

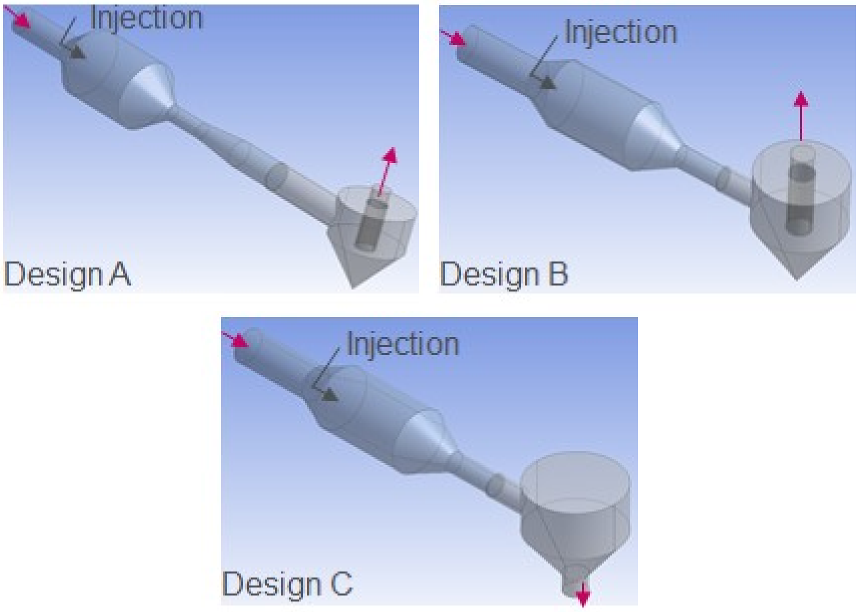


Figure 1. Design candidates tested in CFD modelling; design A, design B and design C

All three designs were composed of two parts which were named injection and expansion pipe and swirl chamber. The injection point was at the axis of the injection and expansion pipe and located just before the expansion section. In this regard, mixing between injected fluid and exhaust gas can be enhanced through the expansion pipe. More specifically, injection fluid molecules will enter the exhaust system whilst the diameter of the pipe is increasing, thus the gap between exhaust molecules also be enlarged and filled with the injected agent. Then, the diameter will again be reduced to increase the velocity before flowing into the swirl chamber, where the turbulence intensity was desired to increase.

The design A had larger expansion pipe diameter, compared to designs B and C. In addition, its exit diameter was the same as the inlet diameter. In contrast, designs B and C had the same injection and expansion pipe dimensions which has smaller exit diameter than exit diameter. The designs A and B had the same swirl chamber with an exit from the top of the chamber. Moreover, the exit pipe extends deep into the chamber, forces the entering exhaust fluid to rotate around it by flowing down (towards the conical part), then flowing towards upside through inside of the exit pipe. By this manner, not only the turbulence intensity but also residence time was desired to improve. On the other hand, the swirl chamber of design C had an exit from the bottom (conical part) of the chamber.

Meshing

The numbers of cells were 492692, 505591 and 485258; and the numbers of nodes were 303136, 265173 and 278201 for designs A, B and C, respectively. Figures 2, 3 and 4 show the meshing for design concepts. Although more accurate results could be achieved with higher meshing size, the results obtained from a similar order of magnitude meshing size would be acceptable [24]. Because the design candidates will only be compared to each other (in terms of turbulence intensity and residence time) to select the best option rather than investigating the NOx reductions.

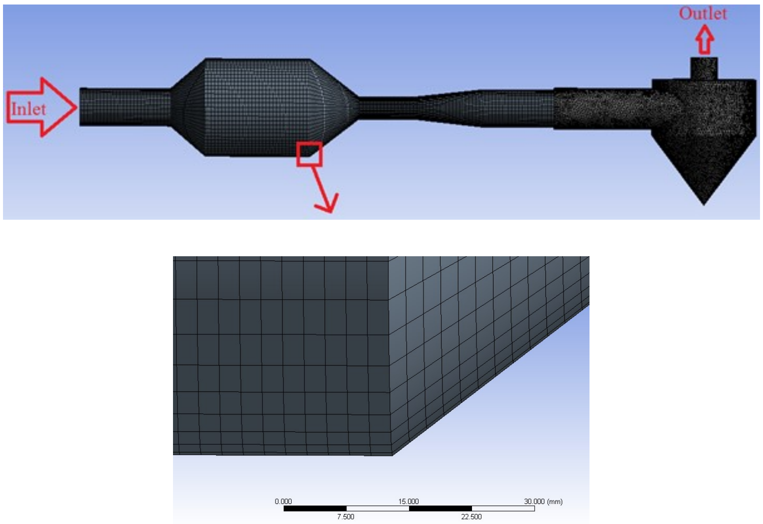


Figure 2. The meshing illustration of design A, which has a larger diameter expansion pipe and venturi between expansion pipe and swirl chamber

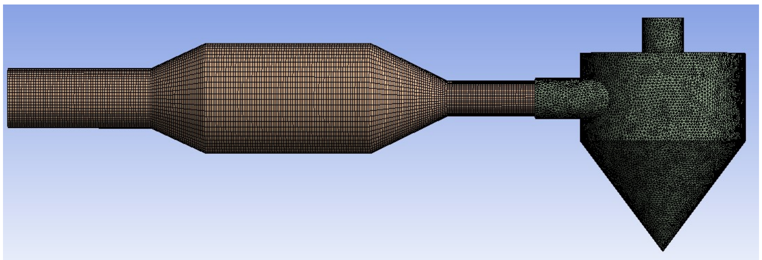


Figure 3. The meshing illustration of design B, which has no venturi between the expansion pipe and swirl chamber and outlet is on top of the swirl chamber.

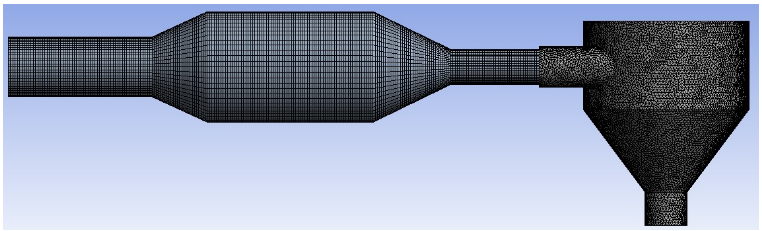


Figure 4. The meshing illustration of design C, which has no venturi between the expansion pipe and swirl chamber and outlet is at the bottom of the swirl chamber

CFD model set up

This simulation was inspired from a CFD modelling for a study aimed for CO_2 emission reduction by magnesium hydroxide injection [24]. All three designs were modelled through the same calculation process, turbulence algorithms and boundary conditions. The viscous – RNG k-e, standard wall functions were selected to have the best monitoring on the turbulence motion [25]. In addition, swirl dominated flow option was selected as it was expected with the presence of the swirl chamber.

Three different species were selected for species model which were assumed as nitrogen oxide as a continuous phase (exhaust gas) and urea-water as a discrete phase. The other exhaust gases were neglected for the simplicity of the study. Nevertheless, the flow behaviour of the exhaust gas can be considered as a single-phase flow, hence neglecting other components was an acceptable assumption for the turbulence intensity and residence time analysis [24].

The discrete phase model was selected for simulating the injection of urea-water solution (AdBlue) into the exhaust gas stream. Interaction with the continuous phase was activated to simulate The evaporation of injection agent and momentum change between the two phases [24]. Then, the injection conditions such as location, direction, nozzle type, temperature, flow rate, injection angle and diameter were introduced to the model. The urea-water option was selected as injection material.

Inlet boundary condition was entered in accordance with the previous experimental measurements [3]. On the other hand, the outlet boundary condition was set as out flow. To provide the interaction between the walls and injected fluid, wall-jet was property was activated. Gravity was also introduced to the model for realistic simulation.

SIMPLE scheme was used for the steady-state flow of pressure related equations; Least Squares Cell Based gradient was implemented for the selected mesh type and minimum false diffusion; PRESTO pressure for swirl flows involving pressure gradients; Second order upwind for more accurate results with Taylor series expansion of the cell-centred solution [24].

CFD model outcomes and design selection

Initially exhaust gas flow was solved without any injection. Then, the injection was implemented too. The system was successfully converged. As discussed earlier, the most important parameters are the turbulence intensity and particle residence time for this selection. The velocity magnitude and turbulence intensities for the design candidates were plotted through velocity vectors and presented in Figure 5. The magnitude scales were arranged the same for all three candidates, hence colour maps of velocity vectors indicate magnitudes of velocity and turbulence intensity. According to results, design A gave much lower velocity and turbulence than designs B and C, thus design A can be eliminated at this stage. However, no significant difference was spotted between designs B and C.

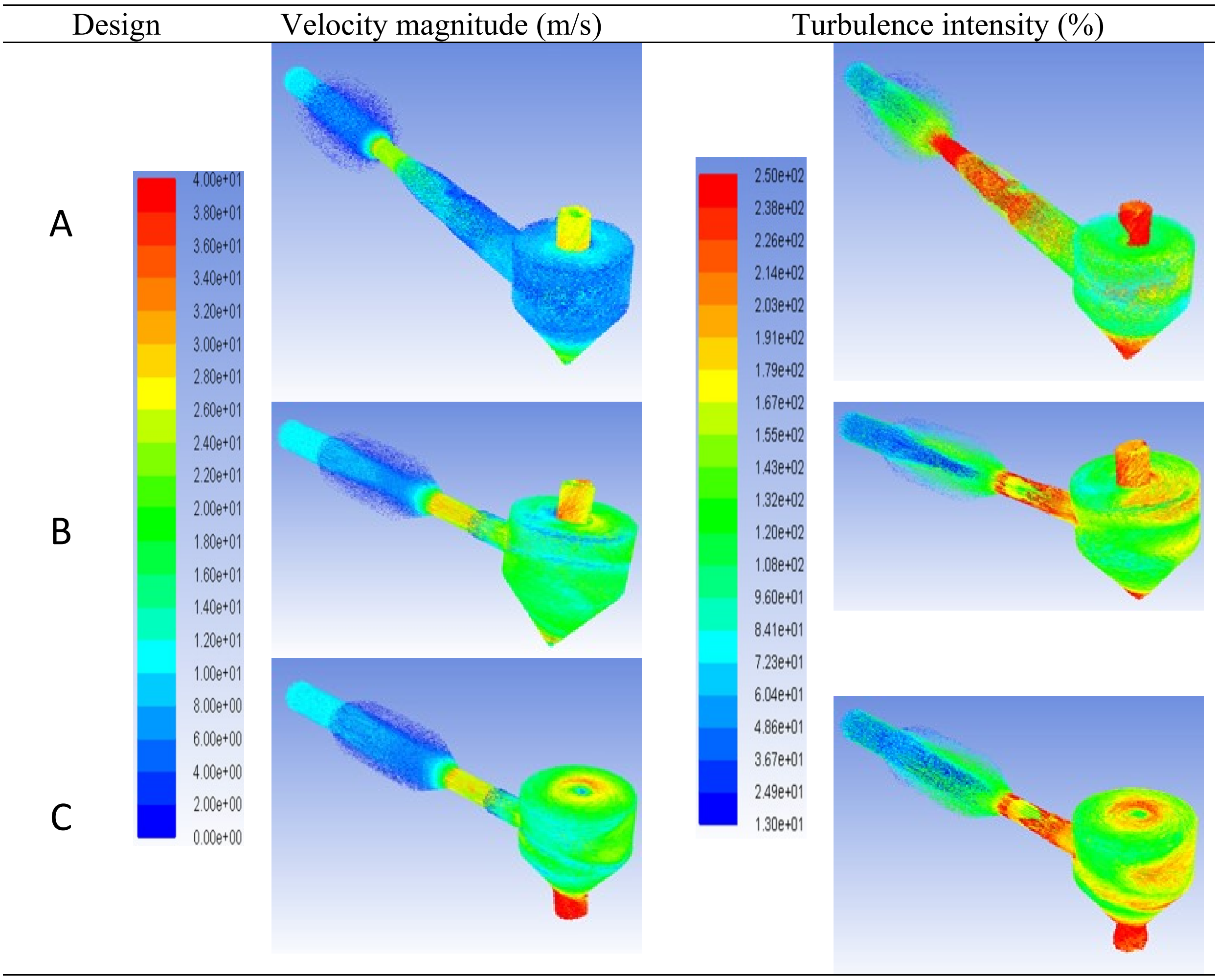


Figure 5. Comparison of design candidates A, B and C in terms of velocity magnitude and turbulence intensity

Design A was eliminated for lower velocity and turbulence, thus designs B and C were compared in terms of particle residence time in Figure 6. The residence time results of design B and C were again comparable at the expansion pipe. However, residence times of the design B and design C were recorded as 3 seconds and 1 second at the swirl chamber, respectively. Consequently, design B was superior to other candidates when all parameters were considered. Therefore, design B was selected to manufacture and conduct the experiment.

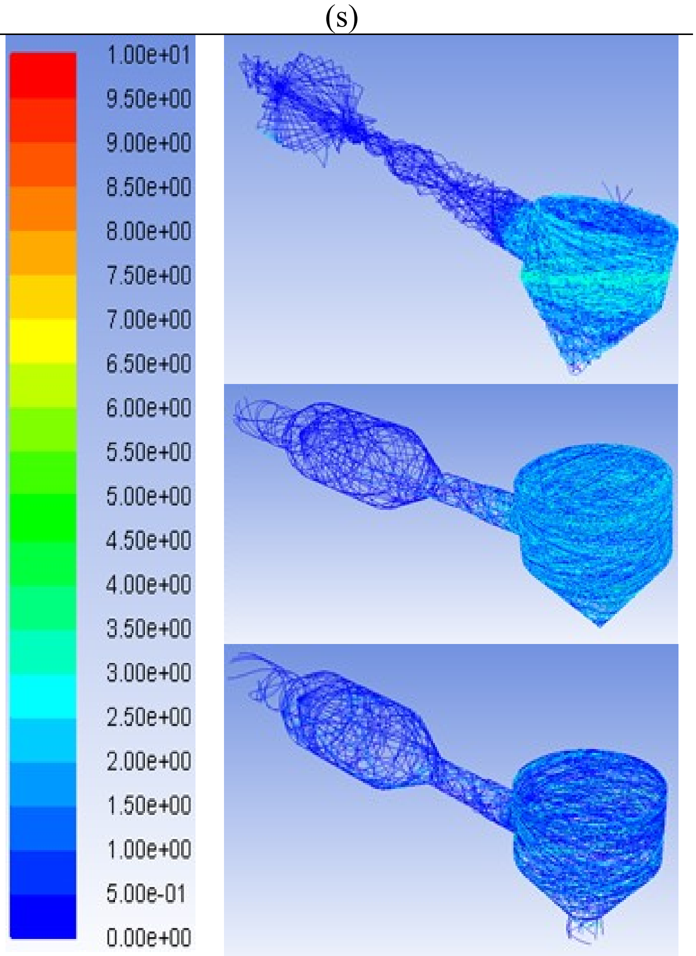
Design candidate	Particle residence time (s)
A	
B	
C	

Figure 6. Comparison of design candidates A, B and C in terms of particle residence time

Experimental investigation of the aftertreatment system

The selected design was manufactured at the duRose Ltd metalwork company in Birmingham. A small water pump and cone injector were used to develop an injection mechanism for the modified SNCR system Figure 7. The flow rate was measured by the stopwatch-bucket method and the lowest flow rate of 375 ml/min was adjusted by providing 3 volts to the pump. Although this value was higher than the calculated value, it was used in the experiment as the NH_3 slip was out of the scope for this analysis.

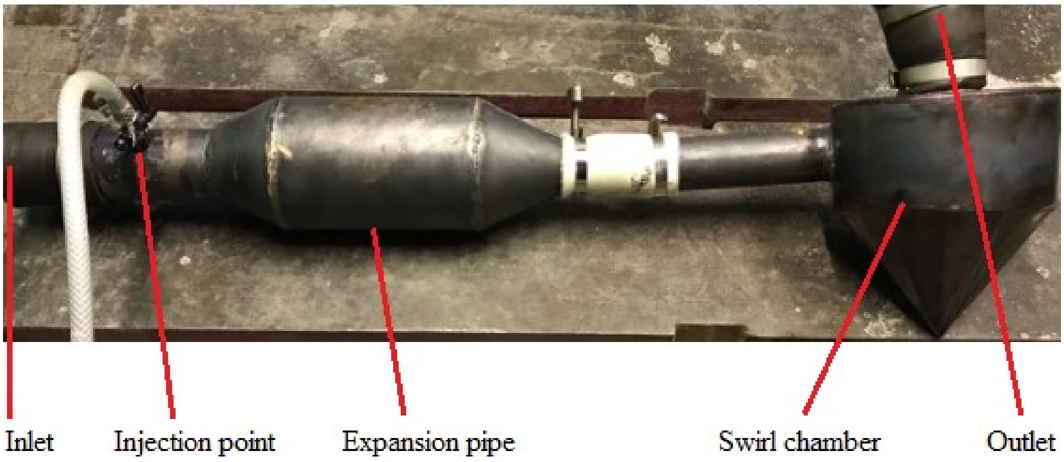


Figure 7. The modified SNCR aftertreatment system assembly

Next, the injector was located into the injection pipe and the flow of the pattern was checked before installing the system on the test rig Figure 8.

Figure 8. Injection pattern starts just before the expansion pipe and expands along with the pipe

The setup was installed on the exhaust system as shown in Figure 9. The national grid power converted into direct current and 3 volts supplied to the pump to reduce the flow rate. The expansion pipe was placed parallel to the ground and the exit of the swirl chamber was located vertically as simulated. The injection was controlled by the on-off switch of the power source. The system was commissioned by a leak test. Moreover, the in-cylinder pressure diagram was checked for any indication of abnormalities due to back pressure. Ultimately, the system was ready for the tests.

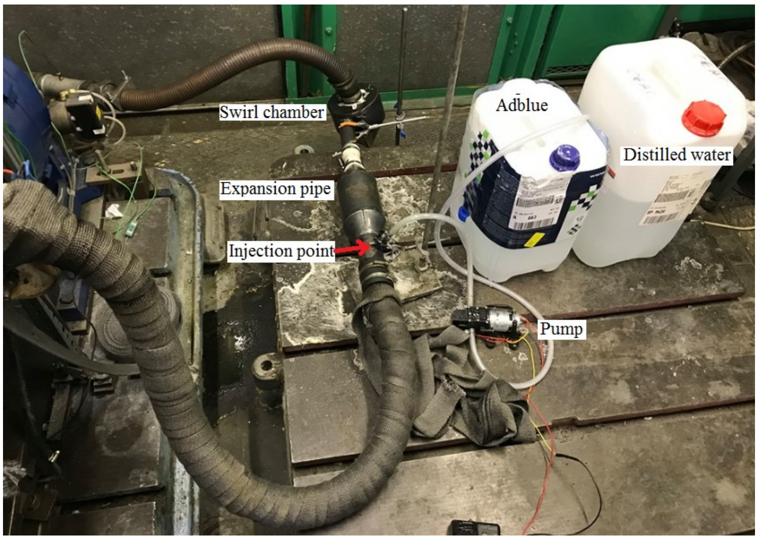


Figure 9. Engine test rig equipped with the modified SNCR after treatment system

RESULTS AND DISCUSSION

In-cylinder pressure diagrams are important to spot any abnormalities regarding the back pressure due to the implemented aftertreatment system [26]. Therefore, in-cylinder pressures of fossil diesel, W50A50 and CO50CH50 were measured at 2000 rpm and at 80% engine load with the modified SNCR system Figure 10. The results gave comparable results with each other such as 67 bars at 13^{o}CA. Moreover, the trends before and after the application of the modified SNCR system were also the same with each other and no abnormal peak or jump was spotted.

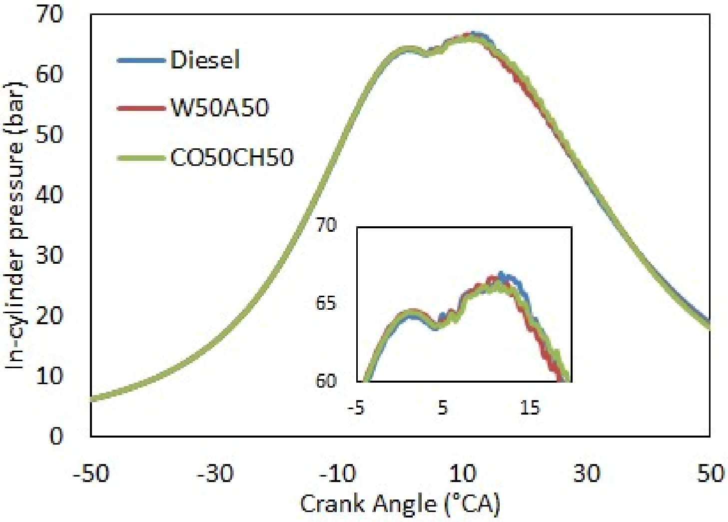


Figure 10. In-cylinder pressures for the test fuels with the modified SNCR aftertreatment system.

CO and CO_2 emissions under no injection, neat distilled water injection and urea-water (AdBlue) injection were given in Figure 11 and 12, respectively. It was clear that there was no significant effect of neither neat water injection nor urea-water injection on CO and CO_2 emissions. This was because there was not any diesel oxidation catalyst (DOC) or diesel particulate filter (DPF) facility on the test rig. However, CO emission was decreased slightly by around 0.006 volume %, 0.005 volume % and 0.003 volume % with the urea-water injection for the diesel, W50A50 and CO50CH50 respectively. CO reduction with urea-water injection was in good agreement with the literature. Praveen and Natarajan [27] also stated a 32% reduction with the urea injection for diesel-ethanol (90/10) blend and linked this reduction to oxidation of CO in the presence of excess oxygen. This also explains the slight increase in CO_2 with urea-water injection.

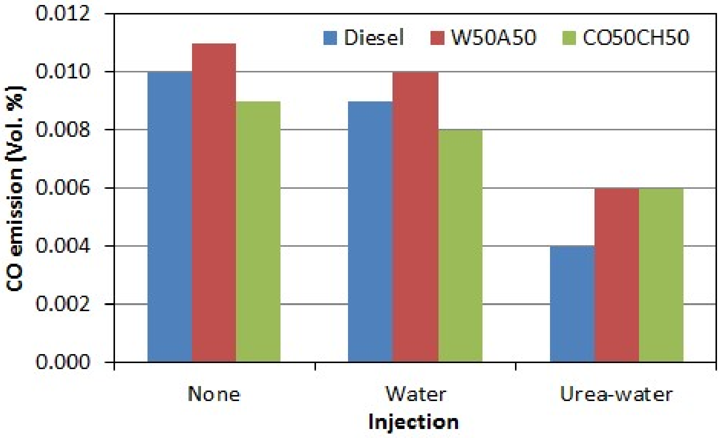


Figure 11. CO emissions of diesel, W50A50 and CO50CH50 with the modified SNCR application.

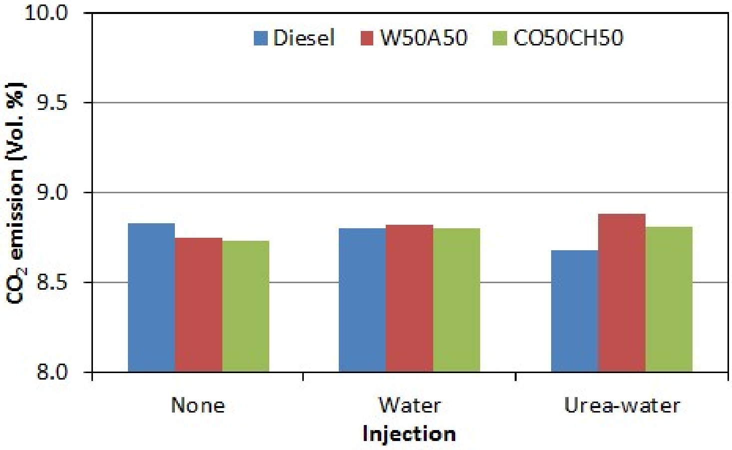


Figure 12. CO_2 emissions of diesel, W50A50 and CO50CH50 with the modified SNCR application.

The unburned hydrocarbons emissions were also measured with and without injections Figure 13. The results were the same in all scenarios; hence HC was not affected by the modified SNCR system. This finding agreed with the literature [17,20].

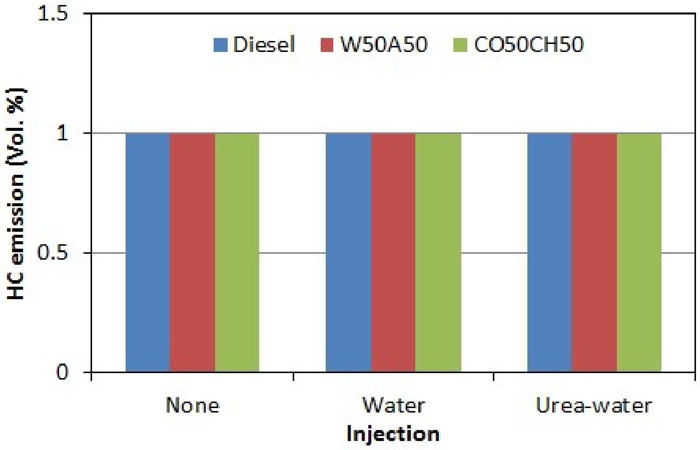


Figure 13. HC emissions of diesel, W50A50 and CO50CH50 with the modified SNCR application.

Figure 14 studies the NO emissions of diesel, W50A50 and CO50CH50 with and without modified SNCR after-treatment system. Without any injection, the biodiesels W50A50 and CO50CH50 gave similar NO emission (at 2000 rpm and 80% engine load) and it was around 1.5% higher than that of diesel. The neat distilled water injection through modified SNCR gave approximately 6% reduction for all three test fuels. Moreover, the urea-water injection reduced the NO emission by 13% and 15% lower than diesel and biomixtures. These emission reductions are likely to be increased for NOx emission, as NO_2 reductions would also contribute to the reduction [8].

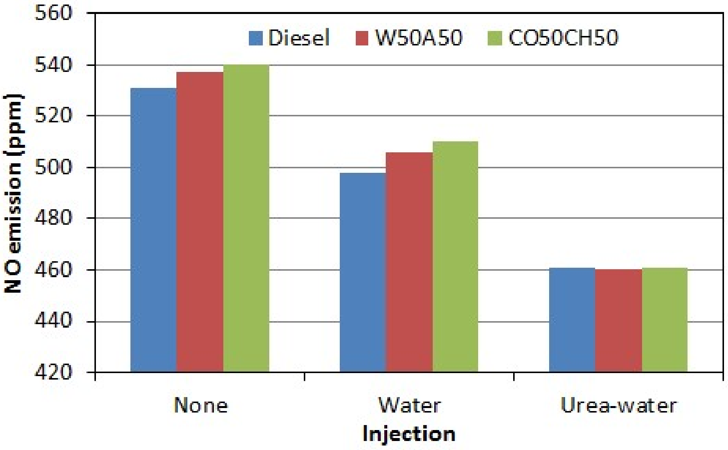


Figure 14. NO emissions of diesel, W50A50 and CO50CH50 with the modified SNCR application.

The modified SNCR aftertreatment system worked without any back pressure problem for low power density engine (11.2 kW at the engine speed of 2000 rpm). The exhaust temperature was observed as 378°C which was well below conventional SNCR temperature window (between 875°C and 1050°C) but above the lower limit of SCR (350°C). Nevertheless, the desired exhaust emission of NO was successfully reduced by 15%. These results proved that the idea of turbulence and residence time improvement through expansion pipe and swirl chamber was successful. Note that this value would be even higher for NOx emission if NO_2 emission could be measured. It is also believed that designed aftertreatment technique would yield further reductions under higher exhaust temperatures with medium or high power density engines.

CONCLUSION

This study focused on NO emission reduction of biodiesels. The latest SCR and SNCR technologies found in literature were combined in a new design to enhance turbulence intensity and residence time. The main advantages of the new system were eliminating catalytic related problems such as weight, clogging, cost etc. The after treatment system was tested in the engine at 80% load with two injection agents which were neat distilled water and commercially available urea-water solution also known as AdBlue. The NO emission of biodiesels and diesel was reduced by approximately 6% and 15% by neat water and urea-water solution injections at 375 ml/min flow rate and at 378°C exhaust temperature. On the other hand, no significant effect of catalyst free modified SNCR system on CO, CO_2 and HC was observed. As a future work, effectiveness of the system can be tested for NO_2 emission and unregulated N_2O emission. Moreover, an advance control mechanism can be developed to minimise NH_3 slip. To illustrate, if upstream NOx emission is measured simultaneously, then an adequate amount of injection fluid can be injected accordingly.

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NOMENCLATURE

CFD – Computational fluid dynamics
CI – Compression ignition
CO – Carbon monoxide
CO2 – Carbon dioxide
CO50CH50 – Cottonseed oil biodiesel and chicken fat biodiesel mixture (50/50 vol.)
$CO(NH_2)_2$ – Urea
DEF – diesel exhaust fluid
DOC – Diesel oxidation catalyst
DPF – Diesel particulate filter
HC – Unburned hydrocarbons
NH3 – Ammonia
NO – Nitrogen oxide
NO2 – Nitrogen dioxide
NOx – Nitrogen oxides
OEM – Original equipment manufacturer
SCR – Selective catalytic reduction
SNCR – Selective non-catalytic reduction
W50A50 – Waste cooking oil biodiesel and sheep fat biodiesel mixture (50/50 volume fraction)

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