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INVESTIGATION OF UREA DECOMPOSITION AND UNIFORM CONCENTRATION OF UREA WATER SOLUTION IN SCR SYSTEM FOR DIESEL ENGINE EXHAUST USING CFD

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ABSTRACT

Urea-SCR has received worldwide attention for reducing the harmful NOx emission from present diesel engines. But this faces lot of challenges such as complete decomposition of reducing agent urea and its deposition at the bottom of exhaust tail pipe, lack of uniform distribution of the urea-decomposed ammonia during the continuous running of the engine. This study is involved with CFD evaluation of urea decomposition rate by adopting different urea injection angles and nozzle positions. Also, urea atomization and evaporation/decomposition to ammonia and ammonia distribution on tail pipe cross-sectional area are investigated. Exhaust tail pipe is fitted with guided pipe at different angles. Also, urea and air are injected at different pressures respectively, in the twin-flow nozzle. The CFD analysis indicated that, the ammonia conversion rate is well improved using guided pipe fitted at 30^{o} inclination with exhaust tail pipe. The CFD analysis is validated by engine experiments. It was proven that, the conversion increased for the 5bar urea and 1bar air.

Keywords: Selective catalytic reduction (SCR); urea-water solution (UWS); ammonia; CFD

INTRODUCTION

Nitrogen oxides (NOx) of air pollutants, obtained from combustion of fossils fuels in thermal power plant, diesel engine and marine vessels, are very dangerous to human health and environment.[1]Reduction of NOx from the engine exhaust up to permissible levels is very much necessary to meet the engine emission standards. There are several techniques available for NOx reduction, such as lean NOx traps (LNT), lean NOx catalyst (LNC), SCR, common rail fuel injection and cooled exhaust gas recirculation (EGR).[2] Usually SCR is a prominent and effective technique for reducing NO_x emissions to nitrogen and oxygen. In SCR a reducing agent is injected into the exhaust pipe[3] for removal of harmful NOx emissions through several steps. Normally H_2, CO[4-6], hydrocarbons[7-9] and urea-water solution (UWS)[10, 11] are the preferred reducing agents.

As soon as the urea-water solution is injected into the exhaust tailpipe, water will evaporate to leave a trail of solid molten urea, which will convert into gaseous ammonia. This conversion of molten urea into ammonia can occur by two steps, namely, thermolysis and further hydrolysis[12]:

Evaporation of water from UWS droplets

$$(NH_2)_2CO\ (aq) \rightarrow (NH_2)_2CO + 6.9H_2O\ (g)$$

Thermolysis of urea into NH_3

$$CO\ (NH_2)_2 \rightarrow NH_3 + HNCO$$

Hydrolysis of iso-cyanic acid into NH_3

$$HNCO (g) + H_2O (g) \rightarrow NH_3 (g) + CO_2 (g)$$

Decomposition of the injected urea is initiated at 133ºC for a very short residence time of 0.1 s [13] and goes to completion at 350°C. [14] To achieve this condition, positioning of the urea injection is crucial; if this position is not proper incomplete urea decomposition may happen. Efficiency of urea mixing and uniformity of urea solution injected into the exhaust gas stream was predicted numerically.[15]

The key factors for higher reduction of NOx are evaporation, decomposition and uniform distribution of reducing agent across the SCR catalyst. This is possible with appropriate design of dosing system which will ensure maximum reduction of NOx.[16] Generally, three strategies are used for the spray formation, namely, airless system, air-assisted internal mixing and air-assisted external mixing. Current urea-SCR systems have their own design and operating conditions but still there could be new ways to improve the performance of SCR. To this effect new design and operating conditions can be incorporated for increasing the efficiency of SCR.[17] CFD methodology can be used for obtaining efficient design and optimized SCR systems. [18] Finite volume method of commercial CFD is used for evaporation and thermal decomposition of UWS for implementing the new design.[19]

In the DeNOx systems a 3D computational model was developed for urea injection and its interaction with the exhaust gas was investigated. [20] Generation and distribution of the urea reducing agent are developed and implemented in the three-dimensional numerical model in the commercial CFD code.[21] NOx of the exhaust gas must react with the ammonia obtained from the injected urea and get reduced to nitrogen and oxygen. This reaction is made easier in the presence of catalysts like MoO_3–CeO_2 Nano Particles[22], Zn-Mg-Al[23], Ni-Mg-Al[23] and Cu-Mg-Al[23], to name a few.

MoO_3–CeO_2mixed oxide nano particles are synthesized by wet chemical method and are coated on ceramic honeycomb, which is used for the NOx reduction.[22] Zn-Mg-Al, Ni-Mg-Al and Cu-Mg-Al have been synthesized by co-precipitation.[23] As well as being nontoxic and inexpensive, these catalysts exhibited increased activity. In this work, effect of different nozzle inlet pressures on urea decomposition was studied using CFD. A small modification in design for uniformity and spray conditions such as injector angle and spray cone angle was made. These findings were validated by experiments using Mn/Ce/Al_2O_3 catalysts.

EXPERIMENITAL

Material and Methods

Mn/Ce/Al_2O_3 catalysts were prepared by one-step sol–gel. In sol-gel method nitrate precursors of cerium (III) ($Ce(NO_3)_3.6H_2O$), aluminium ($Al(NO_3)_3.9H_2O$), and manganese ($Mn(NO_3)_2$, were separately dissolved in ethanol and added together in order to get the different Al:Ce:Mn molar ratio of 1:1:2. The solution was heated at 80ºC and then added drop wise to de-ionized water under constant stirring. After few minutes sols were gradually formed. And cordierite honeycomb samples are prepared by immersing in the sols. Any unclogging of the honeycomb channels by the sols is prevented by air flow using a blower. Then samples were calcined for 2 hours in air at 450ºC.

Catalyst Activity Measurements

Experiments were carried out inconstant speed, four stroke, vertical single cylinder and water cooled Compression Ignition (CI) engine. Test rig specification is shown in Table-1 and the experimental setup is provided in Fig1. The engine is coupled with an SWINGFILED electrical dynamometer to apply 0%, 25%, 50%, 75% and full loads (14 amps). Combustion parameters were measured by AVL pressure transducer fixed on the cylinder head and an AVL 365C angle encoder fixed on the output shaft of the engine. Chromel-alumel (k-type) thermo-couples were fixed for measuring the gas temperature at inlet, exit ducts and cylinder wall. A 50cc graduated burette and stop watch were used to measure the fuel consumption of the engine. Engine speed was determined by a magnetic pick-up sensor connected to a frequency meter. Smoke intensity was measured using an AVL 415 smoke meter. AVL DI GAS 444 exhaust gas analyzer was used to measure the levels of nitrous oxides (NOx), hydrocarbon (HC), carbon monoxide (CO) and carbon dioxide (CO_2) in the emission gas. The fuel injection pressure was maintained at 1 bar throughout the experiment.

Table-1: Engine specification

Type	4-stroke, Vertical cylinder, constant speed, water-cooled, direct injection CI engine
Number of cylinders	One
Cylinder Bore, d	87.5 mm
Stroke length, L	110 mm
Compression ratio, r	17.5:1
Capacity, cc	661.5
Max. power	4.4kW
Rated speed	1500 rpm
Fuel injection	Direct injection
Dynamometer type	Electrical dynamometer
Orifice diameter	13.6 mm
Co-efficient of Discharge	0.6
Injection pressure	220 bar

Fig.-1: Experimental Setup

Numerical Procedure

Computational Domain

Computational flow domain of urea decomposition reactions in the SCR system is as shown in Fig.-2. Two different computational domains are placed the injector – one placed vertically on exhaust tailpipe and other one placed inside a guided pipe which is placed at 30^o to the exhaust tail pipe. CATIA model representing these 2 profiles are shown in Figs.-3a and 3b respectively. Construction of twin-flow nozzle is shown in Fig.-4. In front of the catalytic converter, UWS was injected into the exhaust pipe at different locations of 4.5, 6 and 9inches from the catalytic converter. The SCR reactor was positioned at 11.6 inches from the engine (Fig.-5).

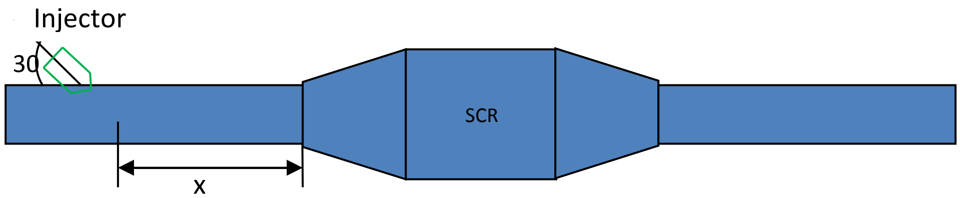


Fig.-2: Computational domain

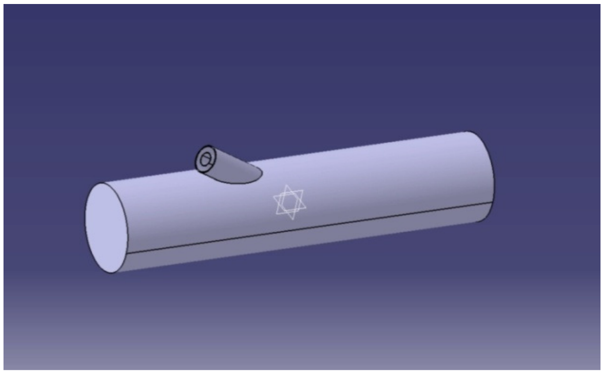


Fig.-3a: 3D Modeling of Exhaust Tail Pipe with 30° inclined guided pipe

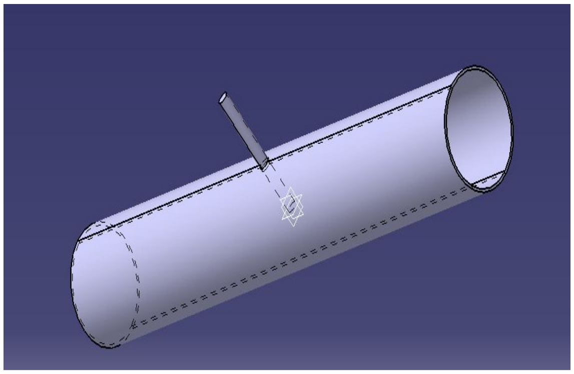


Fig.-3b: 3D Modeling of Exhaust Tail Pipe with vertical positioning of injector

Fig.-4: Cross sectional view of Experimental set up

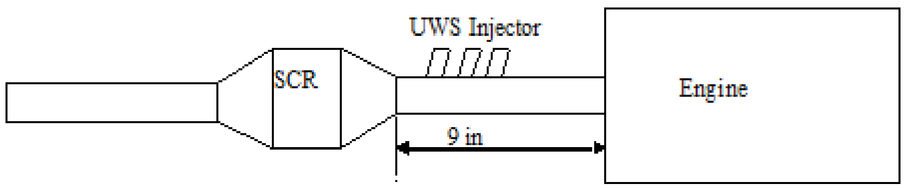
Three-dimensional simulations using different various nozzle inlet pressures are carried out in CFD to investigate the uniform distribution of ammonia at the SCR catalyst entrance. The injector is mounted on the pipe wall along with guided pipe at an angle of 30°. All the numerical solutions are achieved using FLUENT software. The orthogonal grid system used in this work is composed of approximately 4,00,000 cells (Fig.-6), and all numerical analyses are performed by using the same grid system.

Numerical Models

The complicated turbulent flow is solved using k-ω model based on RNG and standard wall functions. The reaction model is validated with the experimental data.

Initial and Boundary Conditions

UWS is injected at different positions of 4.5, 6 and 9inches from the catalytic converter (Fig.-5). Exhaust gas is considered to be composed of 79% N_2 and 21% O_2 in mass fraction. Initial boundary conditions of exhaust gas are listed in Table-2. Outlet pressure is of atmospheric pressure. Exhaust gas is considered to have mean velocity and uniform temperature. Injected particles are assumed to follow uniform distribution.



Note: Position of UWS injector 4.5, 6 and 9inches from the catalytic converter
Fig.-5: Schematic of SCR reactor position and injector position

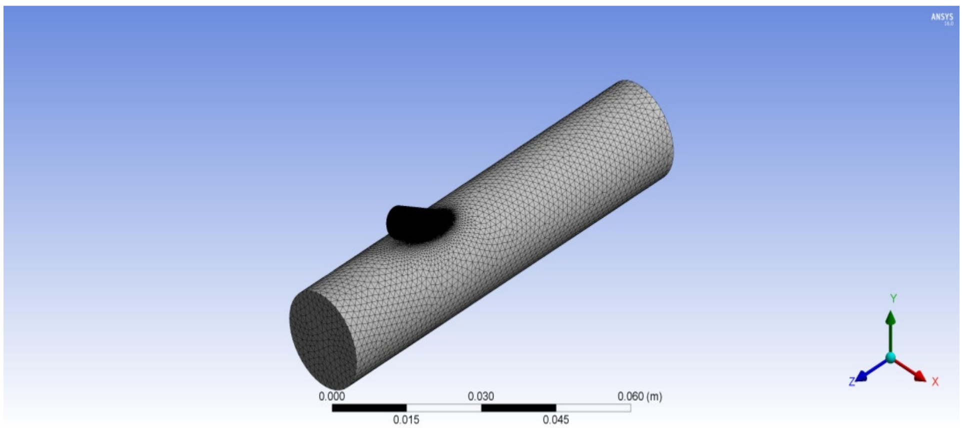


Fig.-6: Mesh of Exhaust Tail pipe

Table-2: Properties of exhaust gas and injector parameters used in simulations

S. No.	Parameters	For full load
Exhaust Gas flow properties		
1	Inlet velocity (m/s)	28m/s (averaged)
2	Inlet Temperature (K)	400K (at full load)
3	The exhaust gas was modeled as air using mole fractions of	21% O_2 and 79% N_2
Injector Parameters		
4	Air dosing pressure	1 bar
5	Urea dosing pressure	5 bar

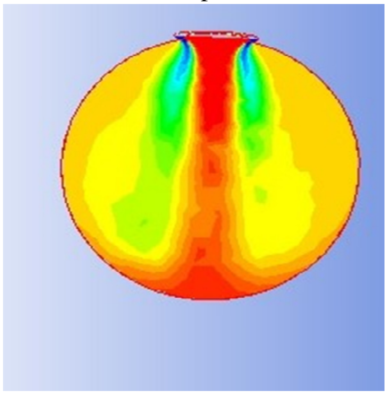
RESULTS AND DISCUSSION

Effect of operational parameters on wall deposition

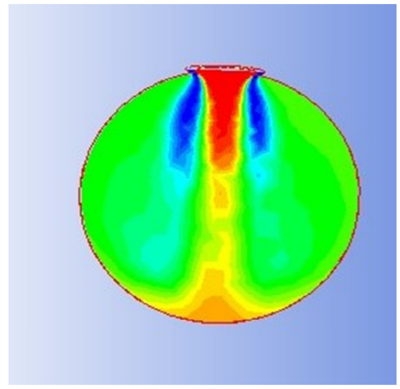
Urea concentrations in the wall film for different operating conditions of twin flow nozzle are shown in Fig. 7. In the main impact area of the spray, the urea concentration is dominated by the urea fraction of the impinged droplets. As the UWS is injected from the injector, case 4 (5 bar UWS and 1bar air pressure) shows less spray impingement. This is because of rapid evaporation of water of UWS leading to instantaneous urea thermolysis/decomposition and thus, prevention of any urea deposition in the tail pipe[4].

2 bar Air pressure

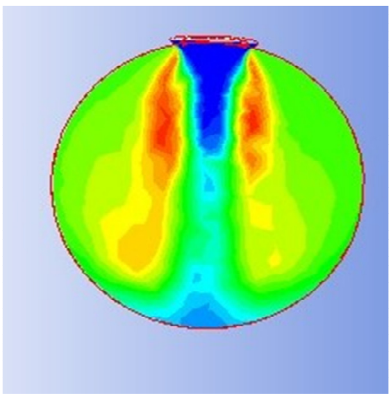
1 bar Air pressure



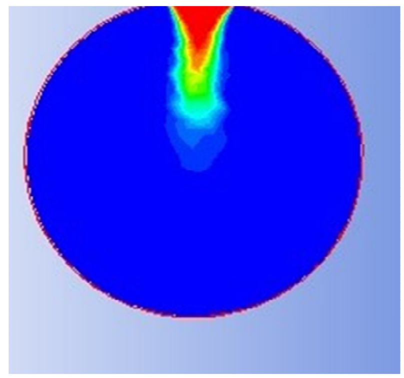
Case 1: 2bar UWS solution



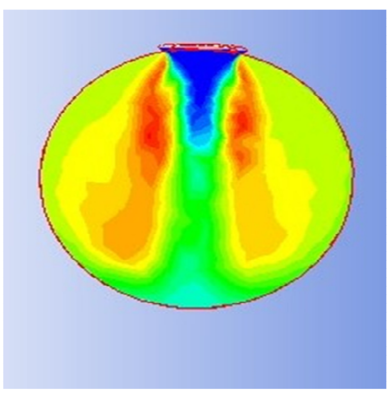
Case 2: 3bar UWS solution



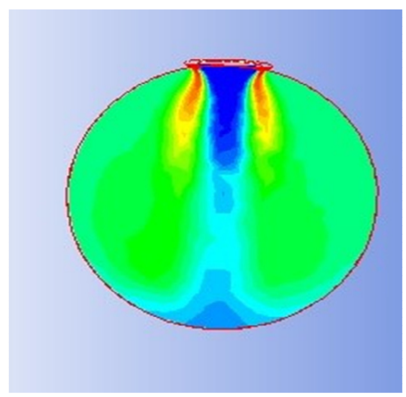
Case 3: 4bar UWS solution



Case 4: 5bar UWS solution



Case5: 6bar UWS solution



Case 6: 7 bar UWS solution

Fig.-7: Urea concentration for different operating parameters

Effect of Ammonia Distribution for Different Geometry

Figures-8 and 9 show the profile of ammonia distribution in the tail pipe for the vertical injector positioning and 30° injector positioning, respectively. For the vertical positioning, poor ammonia distribution and maximum ammonia slip are seen (Fig.-8) which may lead to poor de-NOx efficiency. Poor penetration of UWS up to bottom surface is also noted. For the inclined positioning of Fig.-9, the NH_3 profile exhibits two regions, (i) first region being near the Injector and (ii) second region being away from the injector (front side of catalyst filter in the reactor). It can also be seen from Fig.-9, that, ammonia conversion is dramatically increased as the UWS passes through these two regions. In the first region, case 4 shows highest NH_3 conversion. In the last region, all the cases indicated high ammonia conversion rate which can be due to high pressure in catalyst filter (5 bar UWS) and high residence time (1 bar air pressure).[8] It is concluded that the low air pressure from the nozzle improves residence time. Then, the hydrolysis process is speeded up, and because of this, large amount of NH_3 is generated.[11]

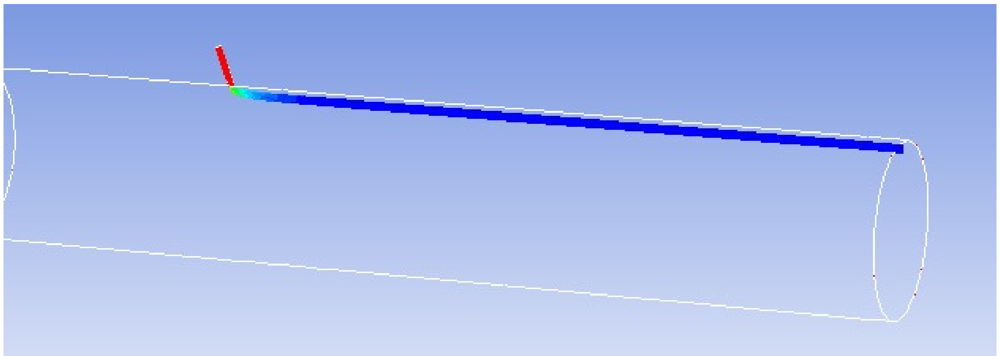


Fig.-8: NH_3 conversion for computational domain 1

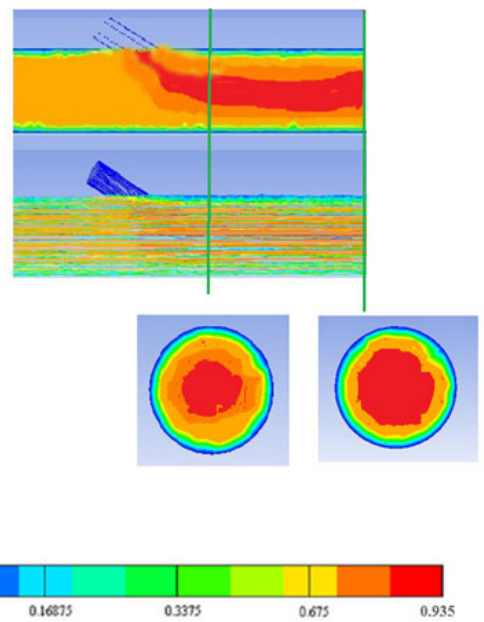


Fig.-9: NH_3 conversion for computational domain 2

Effect of coatings on NOx Reduction

Fig.-10 shows the variation of NOx emission for 13.5%, 18% and 19% of Ce:Al:Mn catalyst loadings on ceramic substance with the injection of 32% concentration urea solution by varying injector angles 30^o at flow rates of 0.8 l/h. It is observed for all the engine load conditions that, there is a significant reduction in NOx in the presence of catalytic converter compared the condition without catalytic converter. Increase of engine load increases NOx production demanding more of urea injection. At engine full loads, NOx reduction was minimum for 13.5% catalyst loading and maximum for 19% catalyst loading. For all these catalyst loadings, NOx reduction was enhanced at 9 inch position of the injector. Vertical injector shows poor NOx reduction compared to that of the 30^o injector. 9 inch position of the injector will give more urea residence time so that, ammonia conversion is enhanced. 30^o injector position will give uniform concentration of ammonia and will prevent deposition of UWS on the tailpipe.

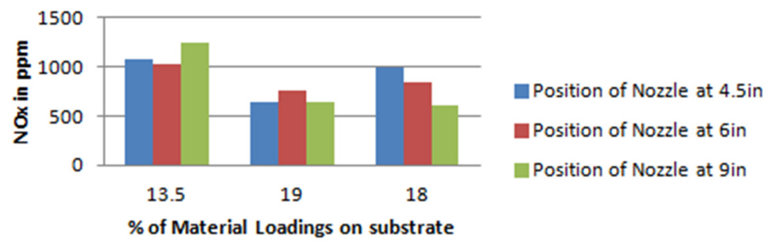
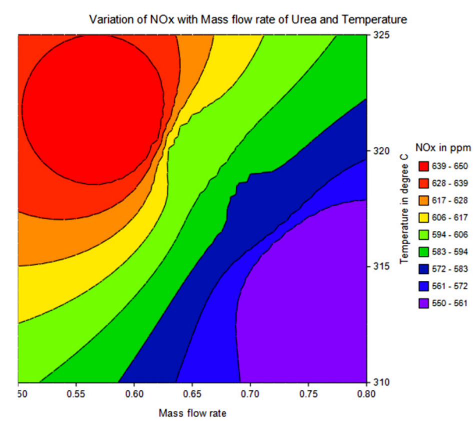


Fig.-10: Variation of NOx at Full Load Conditions for 30^o inclined Position Nozzle

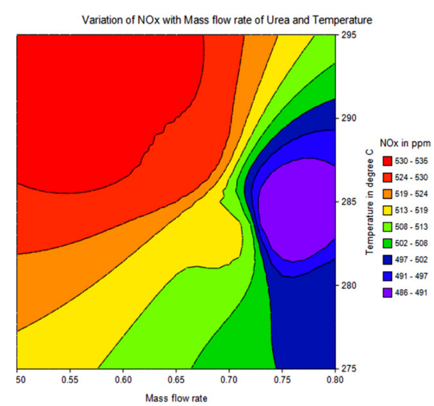
Effect of variation of mass flow rate and temperature on reduction of NOx

Figure-11 shows the variation of exhaust gas temperature at different mass flow rate for a constant 32% UWS and 30^{o}injector angle. Increased engine loads lead to increased exhaust gas temperatures. For the flow rate of 0.8l/h urea solution, a higher NOx reduction was attained at temperatures of 310^{o}C and also at a higher 325^{o}C. Such a high reduction is possible because of adequate amount of ammonia present in the exhaust gas. It may be inferred that higher UWS flow may not be required.

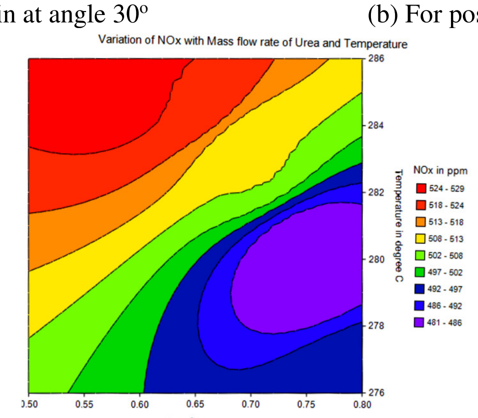
The maximum reduction of NOx (500 to 600 ppm) is achieved for position of 9in from catalytic converter at angle 30^o at the flow rate of 0.8 l/h even at lower temperature less than 276^{o}C. It may be inferred that 9 in position is the best position and 0.8 l/h is the best flow rate.



(a) For position: 4.5in at angle 30^o



(b) For position: 6in at angle 30^o



(c) For position: 9in at angle 30^o

Fig.-11: Variation of exhaust gas temperature with different mass flow rate of constant concentration of urea water solution at 32% and with varying location at 30^o angle

CONCLUSION

Effects of operational parameters on NOx reduction in diesel engine are studied using CFD and also validated by experimental studies. Urea slip is minimized by using different geometrical position of Nozzle. Two regions in SCR are considered for analyzing the NH_3 conversion rate. The first region is near the injector and the second region is farther away from the injector. However, it is found that NOx conversion rate is well improved using guided pipe fitted into exhaust tail pipe at 30^o inclination. And NOx conversion increases for 5bar UWS pressure and 1bar air pressure due to the increased residence time.

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