IJISET - International Journal of Innovative Science, Engineering & Technology, Vol. 4 Issue 6, June 2017
ISSN (Online) 2348 – 7968 | Impact Factor (2017) – 5.264
www.ijiset.com

NOx Aftertreatment Using Urea SCR for Tier 4 Final Application

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Abstract

The paper discusses the optimization of a compact closed coupled Diesel oxidation catalyst + Mixer + Selective catalytic reduction system, complying with Tier 4 final off - road emission legislation. Our paper is based on worst case scenario where the mixing system upstream the SCR catalyst is short and straight pipe which is a challenge in terms of urea conversion and flow mixing. To obtain an enhanced SCR performance, the mixing pipe in this analysis is complemented with three different static mixers. Selection of optimum mixer design is based on interaction between the spray, the turbulent flow field and the mixer element. The performances of different SCR inlet cone designs have been evaluated by predicting the outcome through CFD simulations. Maximum ammonia utilization of 93% was able to achieve at SCR reactor with minimum back pressure.

Keywords: *Static Mixer, Turbulent flow field, Ammonia utilization, Minimum back pressure*

1. Introduction

Computational Fluid Dynamics (CFD) has been an important tool for designing and developing exhaust gas aftertreatment system in the automotive industry. The process of evaluating the SCR performance experimentally by measuring the NH_3 concentration at the inlet of the SCR catalyst is a difficult task that is both expensive and time consuming. However, numerical methods and computational technologies are developed rapidly which enables CFD simulations to predict the atomization and chemical reactions taking place in a SCR system along with flow mixing. Hence, by predicting the flow uniformity through CFD simulations the time for development progression has declined significantly [1].

In a urea SCR system, a urea-water solution often referred to as AdBlue is sprayed into the hot exhaust stream. The AdBlue solution contains 32.5wt% urea and 67.5wt% water. The generation of ammonia (NH_3) in the SCR system is preceded into two steps as described in reactions 1-2. In the first reaction, water (H_2O) evaporated from Adblue droplet and urea $(NH_2)_2CO$ is decomposed to ammonia (NH_3) and iso-cyanic acid (HNCO) through Thermolysis. In the second reaction, HNCO react with H_2O to form another one molecule of NH_3 through Hydrolysis.

1. Thermolysis of urea into NH_3 and iso-cyanic acid

$$(NH_2)_2CO \text{ (s or aq)} \longrightarrow NH_3 \text{ (g)} + HNCO \text{ (g)}$$

2. Hydrolysis of iso-cyanic acid

$$HNCO \text{ (g)} + H_2O \text{ (g)} \longrightarrow NH_3 \text{ (g)} + CO_2 \text{ (g)}$$

In the present Tier 4 application, the space inside cabin is very limited. This means that for a compact SCR aftertreatment applications there may not be sufficient space to obtain both a high conversion of urea and a good mixing of NH_3 and NO_X before the catalyst inlet is reached, meaning that the mixing system where the injection of AdBlue, decomposition of urea and mixing takes place has to be very compact. Regardless of the application, the amount of released NO_X has to be within the allowed level.

2. Problem Definition

The problem is to design a compact type SCR for an off - road vehicle Tractor division which is expected to be Tier 4 - Final emission legislations complaint. The SCR must meet the ammonia flow uniformity acceptance criterions of above 0.95 as set by the exhaust manufactures. The ammonia flow uniformity is optimized by applying various mixer elements & SCR inlet cone design iterations which will be evaluated using CFD code Star CCM+.

The SCR that is under development is planned to be used on a 3 cylinder high pressure common rail diesel engine which has 3.53L engine volume. Figure 1 shows the vehicle parts that are close proximity with exhaust aftertreatment device. As seen in figure 2, SCR will be placed between turbocharger outlet flange and exhaust muffler inlet flange. The SCR, therefore substrate needs to be positioned and designed in a way that adequate clearances must be met to surrounding components such as CRDI line, Intercooler pipe, air filter unit, cylinder head, etc. besides meeting targeted ammonia flow uniformity. Otherwise there is a high risk of overheating of adjacent vehicle components which means either decrease in performance of those components of permanent damage to those components that may result in unfunctionality.

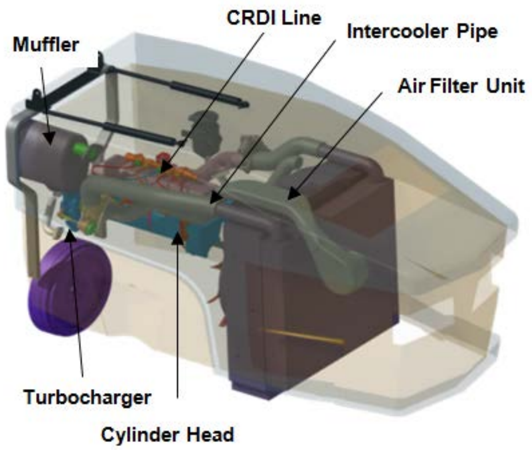

Fig. 1. Vehicle underhood parts in close proximity with SCR exhaust aftertreatment system.

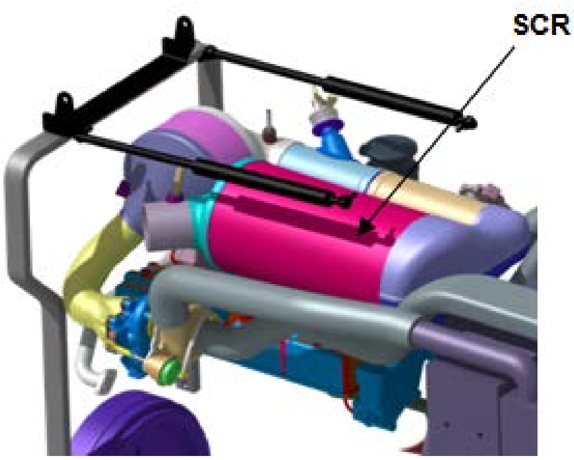

Fig. 2. SCR exhaust aftertreatment package.

3. Ammonia Uniformity Index

To evaluate the mixing performance of the system, uniformity index, UI [3 & 4] is used to quantify the uniformity of ammonia at the monolith entrance as shown in equation (1).

$$\gamma = 1 - \frac{1}{2n}\sum_{i=1}^{n} \frac{\sqrt{(C_i - \bar{C})^2}}{\bar{C}} \quad (1)$$

Where C_i is local concentration of ammonia, $\bar{C}$ is average concentration and n is number of cells.

The mixer and SCR inlet cone design will be accepted as successful if only acceptance criterions applied in exhaust manufactures given in Table 1 are achieved.

Table 1. SCR NH_3 Gamma value acceptance criterions.

Converter Type	NH3 Gamma Value
SCR	≥ 0.95

4. Simulated Injector

Injector sprays Urea Water Solution (UWS) in the exhaust tube. The type of injector used in the simulations is a “solid cone” with a spray angle of 16°, i.e. angle b in Figure 3. The principle direction of the spray diverge 45° from a straight injection, i.e. angle 'a' in Figure 3. Positions and location of the injector were kept constant because of packaging constraints. The droplet diameters are determined by the Rosin Rammler distribution function. Details of single point injector specified for the analysis is shown in table 2.

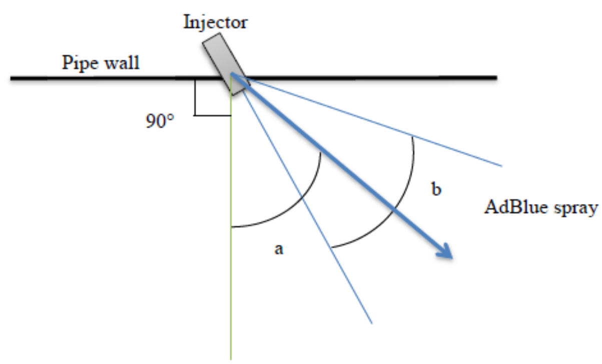

Fig. 3. A schematic figure of injector for the UWS sprays injection.

Table 2. Single point injector details specified in the analysis.

Type	Single point
Mass Flow rate (g/h)	6.3
Particle Temperature (°C)	80
Particle Diameter (µm)	100
Mass Fraction (Urea, Water)	(0.325, 0.675)
Pressure (mbar)	5

5. Boundary Conditions

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The conditions in the system in terms of exhaust gas flow, temperature, UWS flow etc. will vary with the power output from the engine. At some engine power outputs it has been proven to be very difficult to reach high NO_X conversion and will represent a worst case scenario. Therefore such maximum power output has been used in this analysis. The specifications are presented in table 3. Steady State simulation is performed in CFD.

Table 3: Conditions for operating point.

Domain	Type	Value
Inlet	Exhaust Mass Flow Rate (kg/h)	560
	Exhaust Gas Temp (ºC)	660
UWS	Mass Flow Rate (kg/h)	12
SCR	Cell Density (cpsi)	600/4
	Dimension (mm)	Ø 190.5 * 373.38

6. Mixer Selection

Mixing length of (213+57) 270mm shown in figure 4 is provided in the design to have enough time for droplet mixing and evaporation. One of the biggest challenges concerning urea SCR systems is to get efficient vaporization of the urea water solution and get the produced NH_3 evenly distributed. This could be ensured by design optimization of the mixing domain shown in figure 5. Numbers of mixers were varied in the simulations in order to determine the most favorable design. Mixer performance is enhanced by analyzing the maximum turbulent flow with minimum pressure drop. Turbulent flow will enhance to break up the spray into smaller droplets and the evaporation of the urea water solution [5].

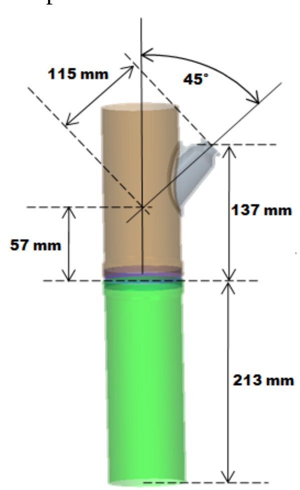


Fig 4. Intermediate mixing pipe for SCR.

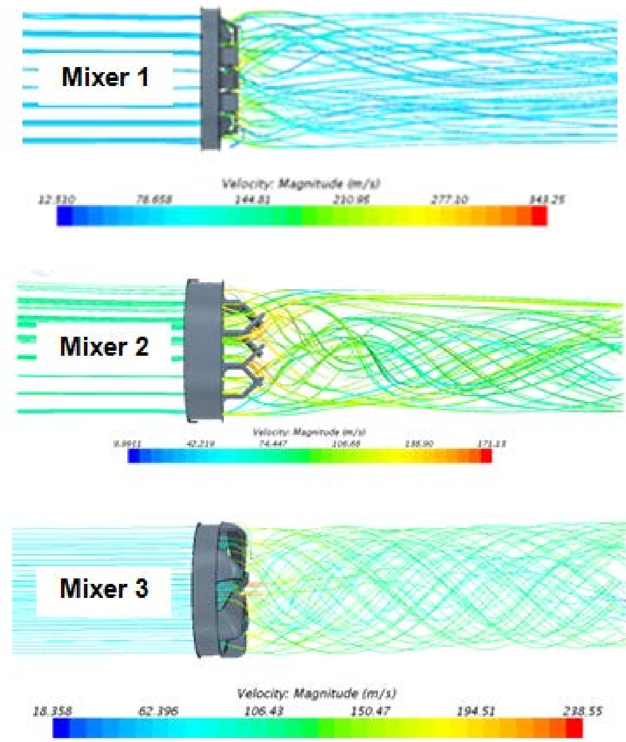
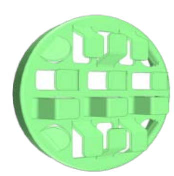
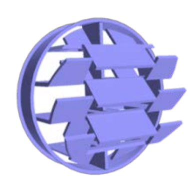


Fig. 5. Streamlines visualizing the effect on the flow field of three different mixers.

Table 4. Different mixer designs.

Mixer 1	Mixer 2	Mixer 3
		
PD = 109.13 mbar	PD = 26.36 mbar	PD = 44.33 mbar

- Mixer 1: Fins projection was initially made perpendicular to the exhaust flow. No Turbulence was produced and backpressure value is very high because of obstructions made in fins.
- Mixer 2: Less turbulence with minimum pressure drop insignificant for droplet mixing.
- Mixer 3: Benchmarked Design of Eberspacher. Each fin was inclined 30º towards the exhaust gas flow. Fine swirl flow were produced which significant for droplet mixing.

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On comparing, the effect of flow field and backpressure value from figure 5 & table 4 respectively. As a worst case scenario, it was decided to perform SCR multiphase flow for both mixer 2 & 3.

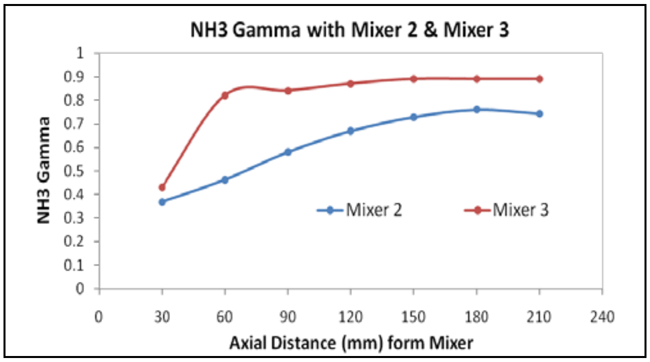


Fig. 6. Comparison of NH_3 gamma value for mixer 2 & 3.

NH_3 gamma value measured across the axial distance from Mixer 3 is high as shown in figure 6. Significance of turbulence ensured proper mixing and evaporation of UWS solution.

7. Proposal and Results

Different SCR inlet cone design iterations with Mixer 3, which are proposed to reach targeted acceptance criterions, are given in details.

7.1 SCR Design Proposal 1

SCR exhaust aftertreatment Design Proposal 1 is built on the Titania Vanadia substrate which has 190.5mm diameter and 373.38mm height. Figure 7 below shows the SCR Design Proposal 1. The aim is to give a half-C shape to the SCR inlet cone in order to distribute the gas uniformly over the substrate to achieve higher utilization, namely higher NH_3 gamma value.

Although this analysis discusses the optimization of SCR inlet cone to achieve ammonia flow uniformity, it is necessary to state that SCR Design Proposal 1 is positioned in a way that it also has optimum clearances to surrounding components. Given this tight package, SCR Design Proposal 1 is designed in a way that gas flow would dissipate over the substrate uniformly.

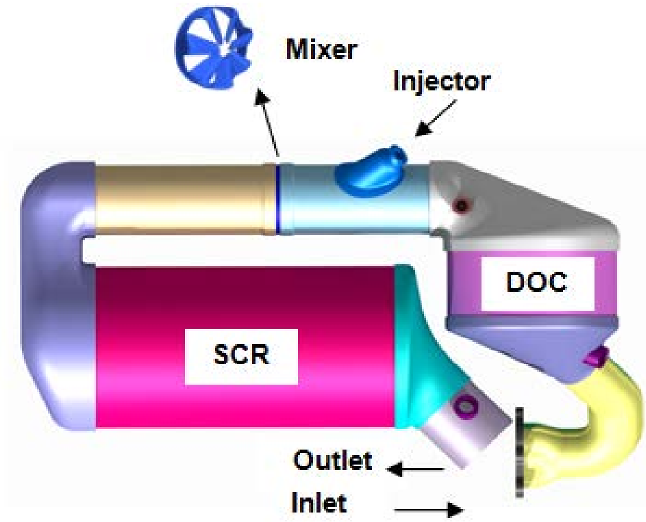


Fig. 7. SCR Inlet Cone Design Proposal 1.

Table 5. Results of CFD analysis for SCR Design Proposal 1.

Attribute	Results	Target
NH_3 Gamma Value	0.68	≥ 0.95

As clearly seen from Table 5 ammonia (NH_3) targets, where the gamma value not met with SCR inlet cone Proposal 1. CFD result plot of SCR inlet cone Proposal 1 is shown on figure 9 below.

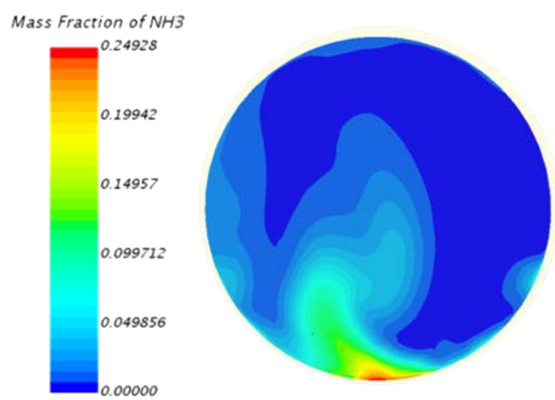


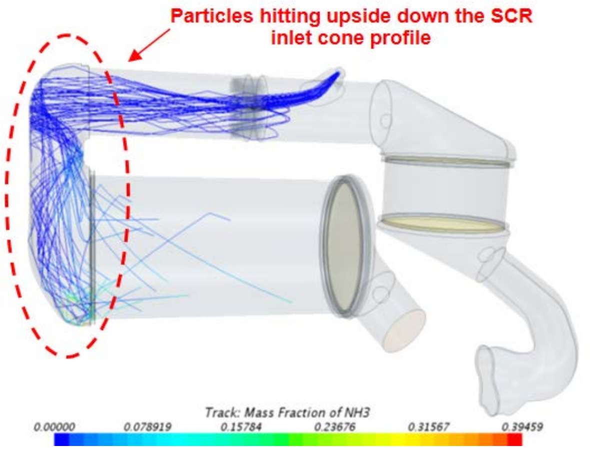
Fig. 8. CFD plot of NH_3 distribution for SCR Inlet Cone Proposal 1.

Assessment of SCR inlet cone Proposal 1 CFD results is:

- NH_3 gamma result of SCR inlet cone Proposal 1 not equals to 1 which indicates very low ammonia gas flow distribution.
- Mass fraction of NH_3 is highly concentrated on the substrate edges. This is also clearly seen from figure 9 above indicated by red color. This indicates there is

high risk of ammonia concentration which jeopardizes useful and durable life of SCR internals, source to urea crystals formation.

- Gamma value of 0.68 indicates that most of the substrate is not being utilized. In other words, ammonia gas flow is highly non-uniform which would probably result in poor emissions conversion efficiency of the SCR.



- Fig. 9. NH_3 particle distribution inside SCR Inlet Cone Proposal 1.
- From figure 9 in dashed spot, it is clearly seen that the particle is taking a trajectory path hitting upside down the SCR inlet cone profile resulting malfunction in ammonia distribution.
- Based on the comments, SCR Design Proposal 1 is considered as not acceptable and cannot be used for the given exhaust aftertreatment system. The necessity of designing a new SCR inlet cone proposal is obvious.

7.2 SCR Design Proposal 2

Inlet cone design Proposal 2 is again built on the same SCR substrate which has 109.5mm diameter and 373.38mm height. Substrate position is kept same with SCR Design Proposal 1 as it has the optimum clearances to surrounding components. Keeping the same substrate position, E shape cone as shown in figure 10 is given to SCR inlet cone Proposal 2. Designing the sheet metal inlet cone in E shape, aim is to increase the ammonia gas flow uniformity after it reaches the substrate evenly.

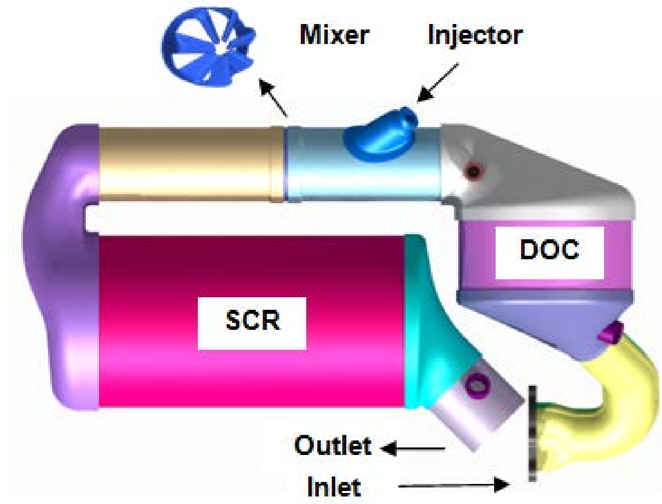


Fig.10. SCR Inlet Cone Design Proposal 2.

Table 6. Results of CFD analysis for SCR Design Proposal 2.

Attribute	Results	Target
NH_3 Gamma Value	0.93	≥ 0.95

As clearly seen from Table 6, Ammonia (NH_3) gamma Value targets are not met but improved 93% with SCR inlet cone Proposal 2.

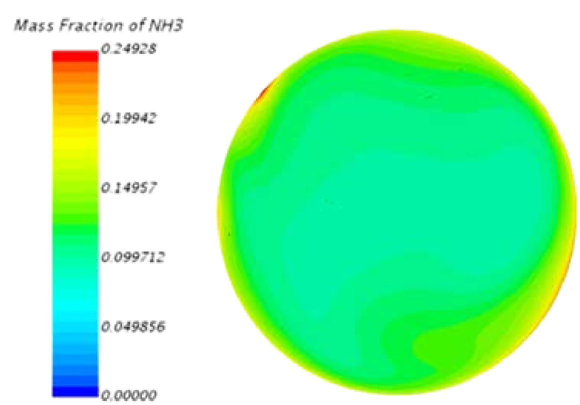


Fig. 11. CFD plot of NH_3 distribution for SCR Inlet Cone Proposal 2.

Assessment of SCR inlet cone Proposal 2 CFD results is:

- Even though NH_3 gamma value is increased to 0.93 by SCR inlet cone Proposal 2, there is still a part of the substrate which is not being utilized as shown by yellowish color on the CFD plot of SCR inlet cone Proposal 2 above. In other words, ammonia gas flow is still not completely uniform.

- The risk of NH_3 slip is reduced compared to SCR inlet cone proposal 1.

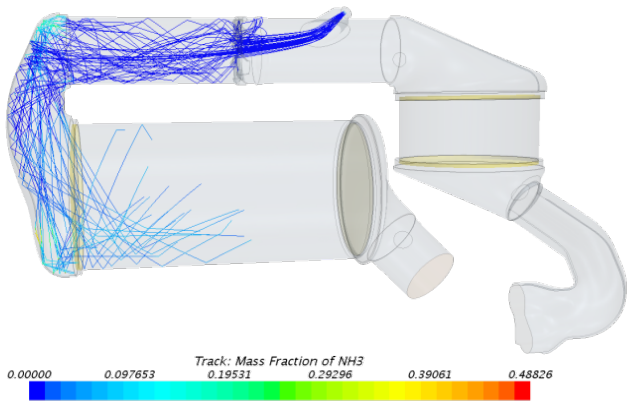


Fig.12. NH_3 particle distribution inside SCR Inlet Cone Proposal 2.

From figure 12, it clearly seen that the ammonia particle now follows the trajectory path of SCR inlet cone and distributes uniformly at SCR substrate.

8. Conclusion

- A three dimensional finite volume (FV) technique applied to optimize SCR aftertreatment system is presented. The paper also accounts for all relevant physics and chemical effects required to simulate SCR simulations.
- Strategy to select optimum mixer, an interactions between different mixing element & turbulent flow field effects saves computational time and best mixer with maximum NH_3 uniformity were able to achieve for the whole exhaust geometry.
- Within given packaging constraints maximum NH_3 Gamma value of 0.93 were able to achieve.
- The possible modifications of the SCR inlet cone are physically limited by a surrounding intercooler pipe and air filter unit positioned between the SCR inlet cones. Thus it is not possible to position further SCR inlet cone designs inside the given package. Therefore, SCR Design Proposal 2 with maximum ammonia gamma value 0.93 is considered as the optimum design.

9. Future Work

- In order to increase the accuracy of SCR simulations, conjugated heat transfer and the liquid film model will include in future investigations with SCR Design Proposal 2. This would mean that the droplet impingement and the droplet evaporation at the wall can be simulated more correctly giving a more complete description of reality.
- Further, the effect of the turbocharger will be investigated using outlet data from simulations of the turbocharger at different power operating points

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Dr. S Rajadurai, born in Mylaudy, Kanyakumari District, Tamil Nadu, India, received his Ph.D. in Chemistry from IIT Chennai in 1979. He has devoted nearly 35 years to scientific innovation, pioneering theory and application through the 20th century, and expanding strides of advancement into the 21st century. By authoring hundreds of published papers and reports and creating several patents, his research on solid oxide solutions, free radicals, catalyst structure sensitivity, and catalytic converter and exhaust system design has revolutionized the field of chemistry and automobile industry.

Dr. Rajadurai had various leadership position such has the Director of Research at Cummins Engine Company, Director of Advanced Development at Tenneco Automotive, Director of Emissions at ArvinMeritor, Vice-President of ACS Industries and since 2009 he is the Head of R&D Sharda Motor Industries Ltd. He was a panelist of the Scientists and Technologists of Indian Origin, New Delhi 2004. He is a Fellow of the Society of Automotive Engineers. He was the UNESCO representative of India on low-cost analytical studies (1983-85). He is a Life Member of the North American Catalysis Society, North American Photo Chemical Society, Catalysis Society of India, Instrumental Society of India, Bangladesh Chemical Society and Indian Chemical Society.

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