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# Optimal Design of Urea-SCR System for Reduction of NOx in Diesel Passenger Cars†

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Much attention has been paid to reduce NOx in diesel engines so that many technologies for diminution of NOx have been developed for last few decades. Among them, the urea-SCR is well known to one of the most efficient method of reducing NOx emissions in the after-treatment devices of diesel passenger cars and light duty vehicles. In the present work, the computational prediction of internal flow and spray characteristics in the urea-SCR system was carried out by using computational field dynamics (CFD) simulation to evaluate $NH_3$ uniformity index ($NH_3$ UI) and its activation time. The number of nozzle and its diameter, injection directions and mounting positions are most important design factors and they are chosen as the design variables. The optimal solutions are obtained by coupling the CFD analysis with Taguchi method. The $L_{16}$ orthogonal array and small-the-better characteristics of the Taguchi method are used and the optimal values are confirmed to be valid in 95 % confidence and 5 % significance level through analysis of variance (ANOVA). The results show that the optimal values of the $NH_3$ UI and activation time ($NH_3$ UI 0.92) are obtained by 0.96 and 0.063 second, respectively and their values are improved by 4.4 and 37.2 %, respectively, compared with those of the base model.

**Keywords: Diesel engine, Urea-SCR, Computational fluid dynamics, $NH_3$ uniformity index, Taguchi method.**

## INTRODUCTION

It is well known that diesel engines generally have higher efficiency but emit more pollutants such as nitric oxides (NOx) and particular matter (PM) than gasoline engines. Therefore, in the automotive industry, the reduction of emissions from diesel engines has been paid attention for both human health and the environment in the past decade.

One of the promising technologies for the reduction of NOx emitted from diesel engines is urea-SCR, the selective catalytic reduction using urea as reducing agent[1]. In this case, a urea-water-solution (UWS, contains 32.5 wt. % urea in water, AdBlue) is sprayed into the hot exhaust stream in front of the catalyst so that urea [$CO(NH_2)_2$] ideally decomposes into $NH_3$, which is the reducing agent needed to transform NOx to $N_2$ on the catalyst in three steps[2].

The subsequent generation of $NH_3$ proceeds in following steps; water is evaporated from a spray of UWS droplets at first. And the solid phase urea melts at 406 K and then the thermal decomposition of urea into gaseous ammonia ($NH_3$) and isocyanic acid (HNCO) momently.

$$(NH_2)_2CO(aq) \longrightarrow NH_2\text{–}CO\text{–}NH_2(s) + 6.9H_2O\ (g) \quad (1)$$

$$NH_2\text{–}CO\text{–}NH_2(s) \longrightarrow NH_3(g) + HNCO(g), \quad \Delta H = 185.5\ kJ/mol \quad (2)$$

In above equation, the resulting HNCO also produces ammonia by a hydrolysis process:

$$HNCO(g) + H_2O(g) \longrightarrow NH_3(g) + CO_2(g) \quad (3)$$

The technology of urea-SCR has a quite complex chemistry and the efficiency of NOx reduction is strongly dependent on both various design variables and operating conditions so that numerical analysis using computational fluid dynamics (CFD) will be an efficient tool for predicting the transport phenomena and obtaining optimal design in exhaust system. According to this reason, the performances of urea-SCR process at a full-scale exhaust system of diesel engines were estimated by computational simulation[3-5].

Recently, Park *et al.*[6] studied numerically the effect of mixer in SCR system on transport phenomena in exhaust system of diesel engines. Multi-phase flow characteristics coupled with chemical reactions were predicted for three dimensional Eulerian-Lagrangian CFD simulation model. They also investigated the influence of mixer on the $NH_3$ reducing rate and the blockage of nozzle for improving the performance of de-NOx system in diesel passenger cars. In

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this study, the performance of urea-SCR system were quantifiable as the $NH_3$ uniformity index (UI) and its activation time.

As mentioned earlier, it is not ease to find studies published on the optimization of the urea-SCR system to improve the de-NOx performance. Therefore, three dimensional Eulerian-Lagrangian CFD simulation to predict the transport phenomena in the urea-SCR system is carried out and multi-phase flow characteristics with turbulent model and various chemical reactions are adopted in the present work. In addition, to obtain the optimal solutions the Taguchi method with the analysis of variance (ANOVA) is adopted and coupled with CFD simulation.

## THEORETICAL ANALYSIS

**Physical configuration:** The physical configuration of urea-SCR deNOx system considered in this study is schematically shown in Fig. 1 and is comprised of the exhaust pipe, urea-injector and mixer. In the urea injector, urea-water solution (UWS) is injected into the hot exhaust gas upstream of the SCR catalyst through the three nozzles and they are collided and mixed at the region of $L_1$-$L_2$. Water of urea-water solution is evaporated first and then the remaining solid state of urea is melted and is decomposed into gas phase ammonia ($NH_3$) and isocyanic acid (HNCO) (region of $L_3$-$L_4$, in Fig. 1).

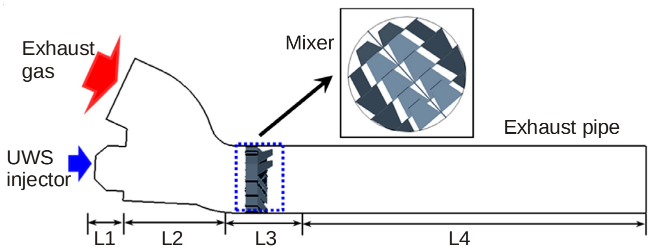


Fig. 1 Physical configuration in front of SCR for the 3-D CFD analysis

**Governing equations:** The transport phenomena occurring inside the urea-SCR system include turbulence, chemical reaction, two phase flow and interaction between the gas phase and reagent droplet phase.

For the prediction of transport phenomena in exhaust gas, the Eulerian framework is used for a continuous phase such as gas. Computational simulation for a continuous phase in the urea-SCR system is carried out by solving the Reynolds-Averaged Navier-Stokes (RANS) equation with the k-ω SST(shear stress transport) turbulence model[7], which can be accurately predict the complex flows with strong adverse pressure gradient and separation. The SST turbulence model is given as follows:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho U_i k)}{\partial x_i}=\tilde{P}_k-\beta^*\rho k\omega+\frac{\partial}{\partial x_i}\left((\mu+\sigma_k\mu_t\frac{\partial k}{\partial x_i}\right) \quad (4)$$

$$\frac{\partial(\rho\omega)}{\partial t}+\frac{\partial(\rho U_i\omega)}{\partial x_i}=\alpha\rho S^2-\beta\rho\omega^2+$$
$$\frac{\partial\omega}{\partial x_i}\left((\mu+\sigma_\omega\mu_t\frac{\partial\omega}{\partial x_i}\right)+2(1-F_1)\rho\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_i}\frac{\partial\omega}{\partial x_i} \quad (5)$$

For computational simulation of the injection phenomena of UWS, the Lagrangian framework for the dispersed phase (in the form of liquid droplet and gaseous) is used in the present work. The transport of the dispersed phase is predicted by tracking the trajectories of a certain number of representative parcels (particles). The momentum conservation equations for a droplet of mass $m_d$ in the Lagrangian framework are as follows:

$$m_d\frac{dU_{i,d}}{dt}=F_{i,d}+F_{i,p}+F_{i,am}+F_{i,b} \quad (6)$$

Here, $U_{i,d}$ is the droplet velocity for i-direction and $F_{i,d}$ is the frag force, $F_{i,p}$ the pressure force, $F_{i,am}$ the virtual force and $F_{i,b}$ the body force.

The atomization of diesel engine fuel spray can be divided into two main processes such as primary and secondary droplet breakup. The primary droplet breakup takes place in the region close to the nozzle of urea injector at high Webber number due to an aerodynamic instability and the Linearized Instability Sheet Atomization (LISA) model[8] is used in this study. The secondary droplet breakup is occurred further downstream in the spray nozzle due to aerodynamic interaction processes and Reitz-Diwaker model[9] is used. According to the model, droplet breakup occurs in both the bag breakup and stripping breakup.

**Numerical analysis:** In the present work, the grid system for the urea-SCR system is constructed by CATIA-V5 CAD file in the ICEM-CFD tetra module[10] and the characteristics of heat and mass transfer are predicted numerically through a general purpose CFD software, STAR CCM+[11] for Eulerian-Lagrangian CFD simulations. Numerical analysis for the exhaust gas with high temperature is carried out first in a continuous phase (Eulerian) and then transport phenomena of urea-water solution (UWS) using a Lagrangian framework for a dispersed phase can be obtained. Computational simulation is also performed by considering the atomization process and chemical reactions such as evaporation of water, thermolysis of urea and hydrolysis of iso-cyanic acid in a Lagrangian framework as shown in eqns. 1-3.

For mesh modeling, tetrahedral and prism layer are used for initial surface (No. of mesh: 27,904) and re-meshed surface (No. of mesh: 98,680), respectively. Finally, the number of volume mesh (polyhedral) is optimized as 466,190 by considering the convergence and the grid system considered in this study is shown in Fig. 2.

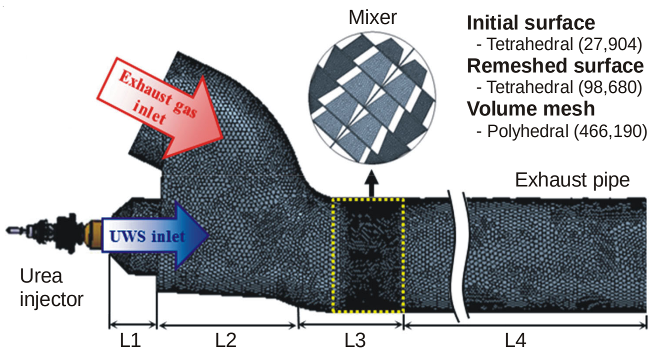


Fig. 2. Grid system for computational domain

The exhaust gas is assumed to be air because the primary objective of this study is predicted the characteristic of UWS behaviour in the urea-SCR system. It enters into the system with a temperature of 300 °C at a flow rate of 39.6 g/s and combined with UWS in the entrance region of the system. The flow rate and temperature of exhaust gas at the inlet region are used by considering the average load of NEDC mode. The UWS (urea: 32.5 wt %, water: 67.5 wt %) is horizontally injected into the exhaust pipe in front of the catalyst through three nozzles at the total flow rate of 0.262 g/s. The nozzles have the same shape and size with diameter of 0.215 mm. The pressure boundary condition is adopted at the exit region and no-slip boundary condition is used in all walls.

## Optimization

In the present work, to acquire a minimized de-NOx of urea-SCR system, shape optimization is carried out by CFD coupled with an optimization technology. The design of variable of urea injector in front of SCR is treated by a design of experiment (DOE) and optimal values are obtained through a smaller the better characteristics of Taguchi method.

**Problem formulation:** A general multi-objective problem is to find the best design variables [X = ($x_i$)], that optimize (*i.e.*, minimize or maximize) several objective functions [$F_i$(X)], simultaneously, subject to a number of inequality [$h_k(X) \leq 0$] or equality constraints [$g_j(X) = 0$] and bounds ($X_r^l \leq X_r \leq X_r^u$). Generally, the feasible design space is defined as the set of all design points expressed by the design variables that satisfy the constraints.

**Objective functions:** The main task of designing the urea-SCR system (*i.e.* exhaust after-treatment system) is to reduce NOx in diesel engines. Generally, the uniformity of $NH_3$ in front of SCR leads to a high de-NOx efficiency because the total surface area of SCR catalyst is effectively used. Therefore, the uniformity of $NH_3$ is chosen as one of the objective functions in this study [$F_1$(X)]. The $NH_3$ uniformity index ($NH_3$ UI, γ) represents the qualitative index whether the transformation of urea-solution to $NH_3$ in the exhaust pipe surface is performed well or not as defined in eqn. 7. As the value of γ is closed to unit, the urea-solution is uniformly transfer to $NH_3$ so that the de-NOx efficiency is improved and the slip phenomenon of $NH_3$ can be dramatically decreased.

$$\gamma = 1 - \frac{1}{2n}\sum_{i=1}^{n}\frac{\sqrt{(\omega_i - \omega_{mean})^2}}{\omega_{mean}} \tag{7}$$

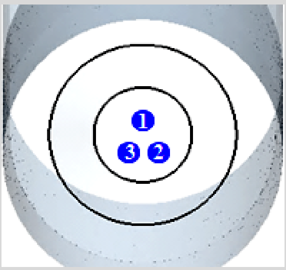
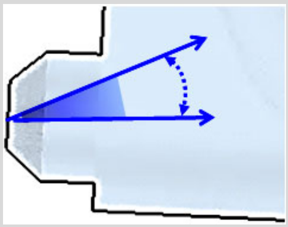
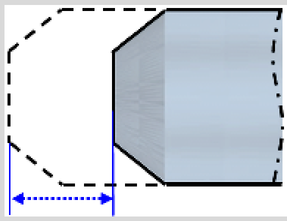
where $\omega_i$ and $\omega_{mean}$ are the local and average concentration values of $NH_3$, respectively and n is the total number of measuring point.

Another important factor for improving the de-NOx efficiency is the activation time to reach the maximum uniformity index of $NH_3$. Gaseous ammonia, which is a reductant of urea-SCR system, is created through the hydrolysis and thermolysis reactions of UWS so that it is generally required an enough reaction time in order to reduce. Therefore, in the present work, the maximum uniformity index (UI) of $NH_3$, $F_1$(X) and the minimum activation time ($NH_3$ UI 0.92), $F_2$(X) are considered as the objective functions.

**Design variables:** For maximization of the reduction efficiency of $NH_3$, many design variables may be considered in the urea-SCR system. It can be possibly achieved the above mentioned two objective functions through the modification of shape and operation conditions of urea injector. Among them, it is commonly accepted that the number of injector nozzle and nozzle diameter, injection angle and injection position influence on the system efficiency. Therefore, in the present work, they are adopted as the design variables and are illustrated in Table-1, in which the constraint conditions are contained.

**Optimization procedure:** The injection strategy for maximization of the deNOx efficiency considered in this work can be determined by optimizing the design variables of urea-injector through a computer aided optimization (CAO) with MDO (multidisciplinary design optimization) method. Fig. 3 shows the overall procedure of optimization. The validation of base model is completed *via* CFD analysis first and then the optimization formula such as the objective function and the design variables with the constraints are performed. The first optimal solution for design variables is numerically obtained by combining the optimization method (DOE) and CFD analysis. If the optimal solutions can not satisfy the maximizing and/or minimizing the objective functions, the design variables and design level are reset by considering the

TABLE-1
CRITICAL DESIGN VARIABLES AND THEIR LEVELS

| | | | |
|---|---|---|---|
| Design variables |  |  |  |
| Base model | 3/0.125 | 20 | 0 |
| Lv. | A: No. of nozzle hole and their diameter (mm) | B: Injection direction (°) | C: Injection position (mm) |
| 1 | 1/0.216 | 0 | -8 |
| 2 | 2/0.153 | 9 | 0 |
| 3 | 3/0.125 | 18 | 8 |
| 4 | 4/0.108 | 27 | 15 |

results of ANOVA (analysis of variance) and CFD simulation is carried out in order to predict the transport characteristics of the system.

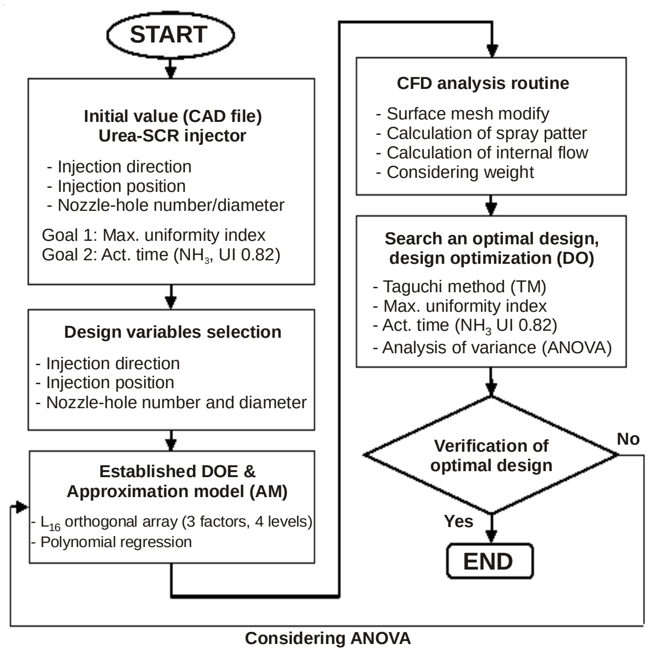



Fig. 3. Overall optimization process

**Design of experiment (DOE):** The uniformity of $NH_3$ density, $F_1(X)$ and the activation time reaching to it, $F_2(X)$, are generally determined by a principle of superposition among the selected three design variables such as the no. of nozzle and nozzle diameter, injection angle and injector position, $X = (x_1, x_2, x_3)$. In the present work, the $L_{16}$ orthogonal array with three factors and $4^{th}$ level are adopted as a design of experiment and it is well known that the orthogonal array method has a good compatibility with various approximated models. Table-2 shows the orthogonal array for the design variables and their level considered in this work.

**Taguchi method[12]:** The DOE of three factors and fourth level can be approached by the smaller-is-better performance which is one of the quality characteristics of Taguchi method. The S/N ratio (signal to noise ratio) which can minimize the expected loss is given by

$$(S/N)_{ratio} = -10\log\left(\frac{1}{n}\sum_{n=1}^{n}\gamma_i^2\right) \quad (8)$$

where n is the number of characteristics and $\gamma_i$ the measured characteristics. For improving the addition of characteristics the 10 log is adopted in eqn. 11 and the minus sign (-) is introduced in order to increase the value of (S/N) ratio as the distribution is small.

## RESULTS AND DISCUSSION

In the present work, numerical analysis is performed to predict the transport phenomena in the exhaust system of small diesel engine for improving the urea-SCR system efficiency.

**Transport phenomena for base model:** As shown in Fig. 1, the hot exhaust gas is mixed with the UWS, which is sprayed at the urea-injector, in front of SCR catalyst within an exhaust pipe and flows by complex flow characteristics in the urea-SCR system. And then, $NH_3$ is produced through the reactions of hydrolysis and thermolysis. In this study, all numerical analysis is carried out for the base model (*i.e.*, the number of nozzle hole: 3, each diameter: 0.215 mm, injection angle: 0 degree and injection position: 0 mm). The mixer is installed at the position of 130 mm from the injector (*i.e.*, the region of $L_3$ in Fig. 1). It is commonly accepted that the installation of the mixer can improve the performance of the urea-SCR system due to the change of flow and thermal fields in the system.

The pressure and velocity distributions for the case of with mixer are presented to compare to those of without mixer as the contours and average values according to the distance from the injector (x/L) in Fig. 4. It can be seen in Fig. 4 that a considerable change of flow field takes place inside the exhaust pipe by the mixer as depicted in the velocity contours. In case of the mixer, the high pressure filed is formed by the back pressure at the region of between the inlet and the mixer and the large pressure drop of 150 Pa is occurred in front of the mixer and it causes the velocity to increase from 7.25 m/s at inlet to 18.34 m/s at mixer exit due to the flow stagnation phenomenon. It is also easily expected that this results in the increase of average temperature (which is not shown in this work). This flow characteristic strongly influences the chemical reaction between UWS and exhaust gas and it impacts on the performance of the urea-SCR system because the vortex flow

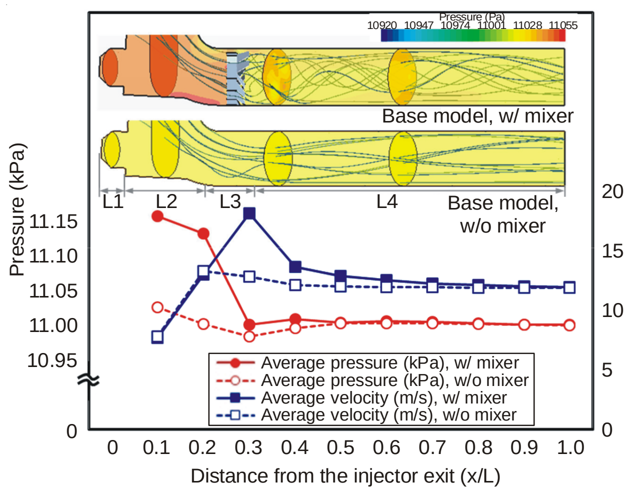



Fig.4. Flow characteristics for the cases of with and without mixer

TABLE-2
ORTHOGONAL ARRAY (L16) FOR THE DESIGN VARIABLES AND THEIR LEVELS

| No | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $x_1$ | 1 | 1 | 1 | 1 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 |
| $x_2$ | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 |
| $x_3$ | 1 | 2 | 3 | 4 | 2 | 1 | 4 | 3 | 3 | 4 | 1 | 2 | 4 | 3 | 2 | 1 |

can promote the mixture rate for them. On the other hand, for the case of without mixer the variation for those variables are predicted as comparatively small (Fig. 4). The fluid velocity at behind the mixer is abruptly decreased due to the vortex which is occurred by the existence of the mixer and then gradually decreased to approach the constant value.

Fig. 5 shows the distribution of uniformity index (UI) of $NH_3$ according to the distance from the injector in order to investigate the effect of mixer on the performance of the urea-SCR system (*i.e.*, reduction efficiency of $NH_3$). The uniformity index of $NH_3$ (γ, UI) which is defined in eqn. 7 is used as the performance criterion of this system and the unit value (*i.e.* 1.0) of UI means that the reduction process is completed by 100 %. As shown in Fig. 5, it looks like almost the same trend until at L = 150 mm from the injector irrespective of the existence of mixer *i.e.*, the UI ($NH_3$) is decreased until the region where exhaust gas and UWS are mixed ($L_2$). And then, for the case of w/o mixer, the uniformity index increases gradually and reaches the maximum value of 0.78 (near at x = 236 mm or x/L = 0.7). On the contrary, the UI ($NH_3$) for mixer is increased abruptly after the mixer and this phenomenon has the same trend as the velocity and pressure distributions as depicted in Fig. 4. Therefore, the UI ($NH_3$) for the case of with mixer is increased by 17.95 % compared to that of without mixer [*i.e.*, the value of UI ($NH_3$) for with mixer is 0.92 (0.16 sec) and for w/o mixer is 0.78, respectively]. This is mainly due to the fact that the mixer leads to the vortex flow and helps to mix between the exhaust gas and the UWS. This flow characteristic results in not only the delay wall-wetting but also the vigorous reactions of hydrolysis and thermolysis in the exhaust pipe. It is also found from the result that the NOx emission effect is increased when the mixer is installed in the exhaust pipe qualitatively. This considerable alteration of performance is caused by the increasing the mass fractions of urea and $H_2O$ (Fig. 6).

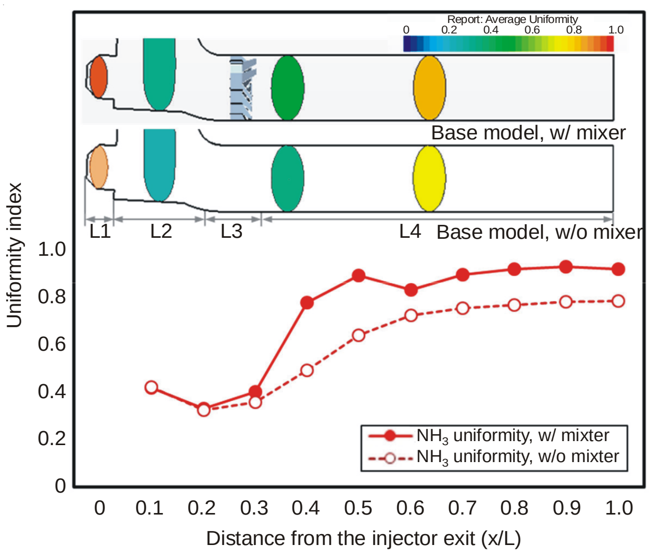


Fig. 5. Uniformity index (UI) of $NH_3$ for the cases of with and without mixer

**Optimal solutions:** Table-3 presents the results of CFD simulation according to the orthogonal array ($L_{16}$). Because the objective functions [max. UI($NH_3$) and min. activation time for max. $NH_3$] have a different unit and dimensions, it is necessary to normalize them to calculate the S/N ratio for the optimization.

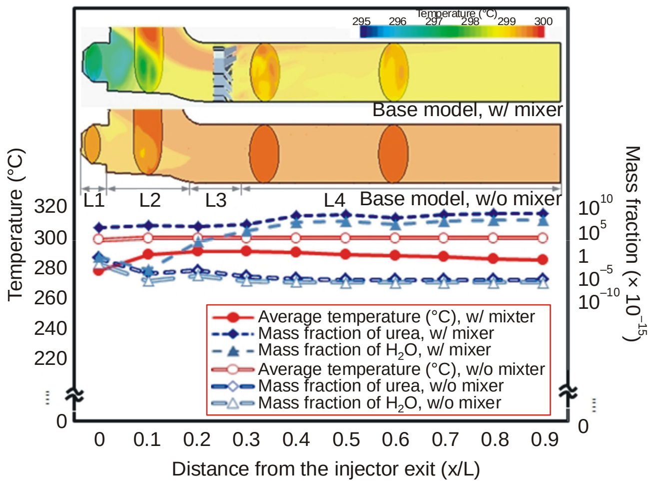


Fig. 6. Average temperature and mass fractions of urea and $H_2O$ for the cases of with and without mixer

TABLE-3
RESULTS FOR CFD SIMULATION ASSOCIATED WITH THE EXPERIMENTS

| No. | Maximum $NH_3$ UI | Act. Time (0.82) (s) | S/N ratio |
|---|---|---|---|
| 1 | 0.901 | 0.0915 | 2.25 |
| 2 | 0.893 | 0.0938 | 1.87 |
| 3 | 0.906 | 0.100 | 1.87 |
| 4 | 0.948 | 0.105 | 2.51 |
| 5 | 0.909 | 0.089 | 2.62 |
| 6 | 0.911 | 0.087 | 2.82 |
| 7 | 0.906 | 0.105 | 1.58 |
| 8 | 0.960 | 0.098 | 3.25 |
| 9 | 0.884 | 0.092 | 1.64 |
| 10 | 0.851 | 0.085 | 0.83 |
| 11 | 0.903 | 0.098 | 1.88 |
| 12 | 0.943 | 0.102 | 2.70 |
| 13 | 0.861 | 0.099 | 0.55 |
| 14 | 0.889 | 0.092 | 1.81 |
| 15 | 0.934 | 0.088 | 3.49 |
| 16 | 0.948 | 0.094 | 3.34 |

Fig. 7 shows the variation of S/N ratio according to the design variables or design levels. It is noted that the maximum value of S/N ratio means the optimal level for each design variable. As can be seen in the figure, the optimal solutions obtained in this study are as follows; nozzle diameter of 0.153 mm ($x_1$), two number of nozzle ($x_1$), injection angle of 27° ($x_2$) and the same position as the base model ($x_3$). The results of analysis of variance (ANOVA) are listed in Table-4, which has the confidence of 95 % and the level of significance of 5 %. As shown in the table, P-values for the injection direction and its position have less than 0.05. However, P-value for the hole number/diameter is estimated as 0.767.

In order to validate the optimal solutions for the design variables obtained in the study, the variation of $NH_3$ uniformity index (UI) for the optimal model according to the distance (x/L) is displayed in Fig. 8 and is also compared with that of the base model. The UI($NH_3$) for the optimal and base models are predicted as 0.96 and 0.92, respectively and the minimum time to reach the maximum UI ($NH_3$) for the base model (*i.e.*, 0.92) is estimated by 0.063 sec. This is due to the fact that the flow

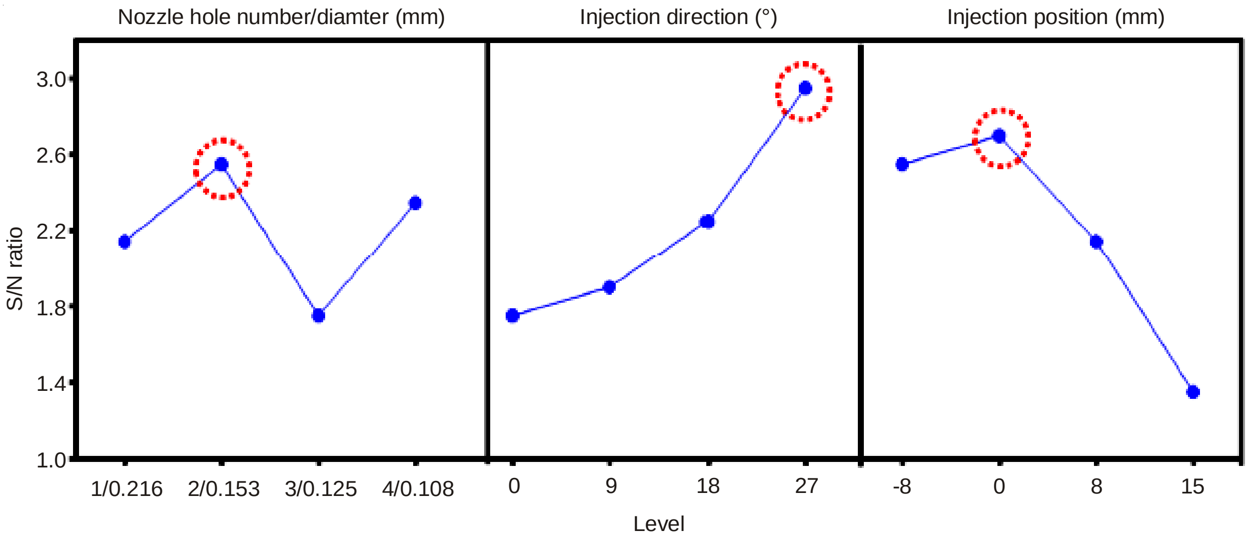



Fig. 7. Optimal level for the design variables by Daguchi method

TABLE-4
RESULTS OF THE ANOVA DISTRIBUTION

| Design variable | Degree of freedom | Sum of square | Mean square | F | P |
|---|---|---|---|---|---|
| No. of hole/dia. | 1 | 0.0710 | 0.0710 | 0.09 | **0.767** |
| Injection direction | 1 | 5.2130 | 5.2130 | 6.72 | **0.024** |
| Injection position | 1 | 3.9613 | 3.9613 | 5.11 | **0.043** |
| Error | 12 | 9.3091 | 0.7758 | – | – |
| Total | 15 | 18.3467 | – | – | – |

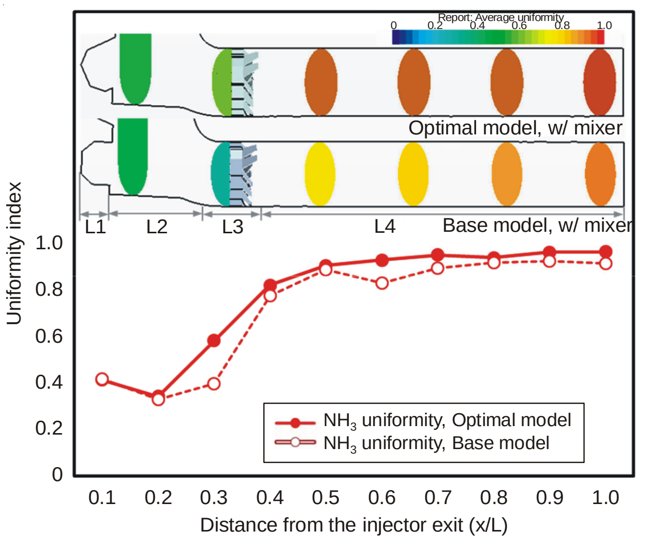



Fig. 8. Comparison of the uniformity index(UI) of $NH_3$ for the optimal and base models

contact area is decreased because of a high position of collision. This phenomenon causes the conversion time to $NH_3$ to grow longer and the accumulation of UWS on the wall to decrease. This result also shows that the conversion efficiency of $NH_3$ for the optimal model and the activation time are improved by 4.4 and 37.2 %, respectively, compare to those of the base model.

## Conclusion

In the present study, numerical analysis has carried out to investigate the performance of urea-SCR system in diesel passenger car, which is one of the promising technologies for the abatement of the nitrogen oxides (NOx) emission. Three-dimensional transport phenomena coupled with chemical reactions in the exhaust system are predicted by a general purpose CFD code of STAR-CCM+ and a multi-phase flow are considered for Eulerian framework for exhaust gas and Lagrangian one for solid phase of urea-water solution (UWS). The number of nozzle, diameter of the nozzle, injection directions and mounting positions are chosen as the design variables. In addition, the adopted objective functions are the $NH_3$ uniformity index ($NH_3$ UI) and the activation time because they are most important factors to verify the performance of de-NOx system in diesel passenger cars. The calculated optimal solutions for the design variables are as follows; the number of nozzle hole is 2 (two), the nozzle diameter 0.153 mm, the injection angle 27° and the injection position 0 mm. It is also found that the maximum $NH_3$ uniformity and the activation time for the optimal model are improved by 4.4 and 37.2 %, respectively, compared with those of the base model.

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