

Numerical Prediction on the Influence of Mixer on the Performance of Urea-SCR System

Kyoungwoo Park, Chol-Ho Hong, Sedoo Oh, Seongjoon Moon

Abstract—Diesel vehicle should be equipped with emission after-treatment devices as NO_x reduction catalyst and particulate filters in order to meet more stringer diesel emission standard. Urea-SCR is being developed as the most efficient method of reducing NO_x emissions in the after-treatment devices of diesel engines, and recent studies have begun to mount the Urea-SCR device for diesel passenger cars and light duty vehicles. In the present study, the effects of the mixer on the efficiency of urea-SCR System (i.e., NH₃ uniformity index (NH₃ UI) is investigated by predicting the transport phenomena in the urea-SCR system. The three dimensional Eulerian-Lagrangian CFD simulation for internal flow and spray characteristics in front of SCR is carried out by using STAR-CCM+ 7.06 code. In addition, the paper proposes a method to minimize the wall-wetting around the urea injector in order to prevent injector blocks caused by solid urea loading.

Keywords—Computational fluid dynamics, Multi-phase flow, NH₃ uniformity index, Urea-SCR system, Urea-water-solution.

I. INTRODUCTION

IT is well known that diesel engines generally have higher efficiency and emit more pollutants such as nitric oxides (NO_x) 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 NO_x 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(NH₂)₂) ideally decomposes into NH₃, which is the reducing agent needed to transform NO_x to N₂ on the catalyst in three steps[2].

Koebel et al. [3] discussed some challenges and selected problems that arose if the SCR process would be adopted to mobile diesel engines. They concluded that the much shorter residence time of the exhaust gas in the catalyst will lead to higher secondary emissions of ammonia and isocyanic acid originating from the reduction agent.

The technology of urea-SCR has a quite complex chemistry and the efficiency of NO_x reduction is strongly dependent on

both various design variables and operating conditions. Therefore, numerical analysis using computational fluid dynamics (CFD) will be an efficient tool for predicting the transport phenomena and obtaining optimal design in exhaust system so that it has been widely used to predict the performance of Urea-SCR process at a full-scale exhaust system of diesel engines.

Jeong et al. [4] numerically studied on the effects of location and number of hole of urea injector on the deNO_x performance of heavy-duty diesel engine. They insisted that the location of injector, the number of nozzle hole, and the injection angle were the important design factors for improving the urea-SCR system efficiency.

Birkhold et al. [5] investigated theoretically the evaporation of water from a single droplet of urea water solution by the commercial CFD code (Fire 8.3) and compared CFD simulation of a SCR de-NO_x system to experimental data to determine the kinetic parameters of the urea decomposition.

Strom et al. [6] investigated droplet-flow interactions in a urea-SCR-spray originating from nozzle located at the exhaust pipe wall to choose the adequate models of urea-SCR systems by considering a very simple and basis system setup(i.e., two-dimensional channel flow) and using commercial CFD software (Fluent 6.3.26). They insisted that only the forces due to drag and buoyancy were necessary in order to correctly describe droplet motion in Eulerian-Lagrangian modeling of the urea-SCR system.

To our knowledge, it is not ease to find studies published on the effects of the operating conditions on the de-NO_x efficiency such as the NH₃ uniformity index and the its activation time for three dimensional Eulerian-Lagrangian CFD simulation by predicting the transport phenomena in the urea-SCR system. In the present work, multi-phase flow characteristics coupled with chemical reactions are predicted numerically and the influence of mixer on the NH₃ reducing rate and the blockage of nozzle are investigated for improving the performance of de-NO_x system in diesel passenger cars. It is also studied on the install location of the mixer in the urea-SCR system.

II. THEORETICAL MODEL

A. Physical Configuration

The physical configuration of urea-SCR de-NO_x 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, urea: 32.5 wt%, water: 67.5 wt%) is injected into the hot exhaust gas upstream of the SCR catalyst through the three nozzles ($d = 0.125\text{mm}$, $m = 0.262\text{g/s}$, $T = 20^\circ\text{C}$) and they are collided and mixed at the

Kyoungwoo Park is with the Department of Mechanical Engineering, Hoseo University, Asan 336-795, Korea (phone: +82-41-540-5804; fax: +82-41-540-5808 ; e-mail: kpark@hoseo.edu).

Chol-Ho Hong is with the Department of Robot Automation Engineering, Hoseo University, Asan 336-795, Korea (e-mail: chhong@hoseo.edu).

Sedoo Oh and Seongjoon Moon are with Korea Automotive Technology Institute, Cheonan 330-912, Korea (e-mail: sdo@katech.re.kr, sjmoon@katech.re.kr).

region of $L1 - L2$. Water of UWS 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 $L3-L4$, in Fig. 1).

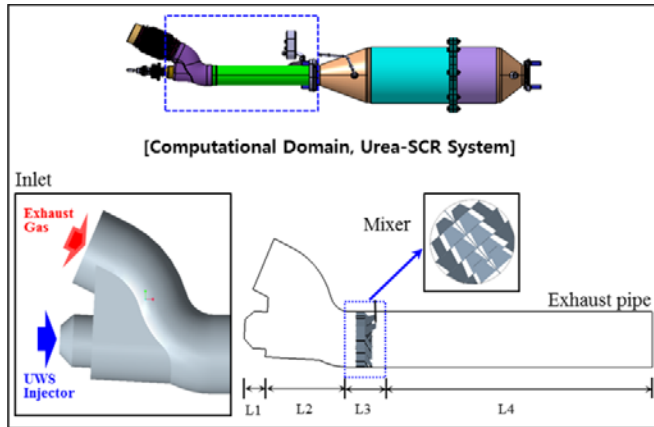


Fig. 1 Physical configuration in front of SCR for the 3-D CFD analysis

B. Governing Equations

All 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 $k-\omega$ 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;

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho U_i k)}{\partial x_i} = \tilde{P}_k - \beta^* \rho k \omega + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_i} \right] \quad (1)$$

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

where blending function F_1 is defined as follow:

$$F_1 = \tanh \left\{ \min \left[\max \left(\frac{\sqrt{k}}{\beta^* \omega y}, \frac{500\nu}{y^2 \omega} \right), \frac{4\rho\sigma_{\omega 2} k}{CD_{kw} y^2} \right] \right\} \quad (3)$$

with CD_{kw} and y is the distance to the nearest wall

The turbulent eddy viscosity is defined by:

$$\nu_t = \frac{\alpha_1 k}{\max(\alpha_1 \omega, SF_2)} \quad (4)$$

where S is the invariant measure of the strain rate and F_2 is a second blending function given by;

$$F_2 = \tanh \left\{ \max \left(\frac{2\sqrt{k}}{\beta^* \omega y}, \frac{500\nu}{y^2 \omega} \right) \right\} \quad (5)$$

In (1), a production limiter (\tilde{P}_k) which is used to prevent the build-up of turbulence in stagnation regions in the SST model is defined as follows;

$$\tilde{P}_k = \min \left[P_k, 10\beta^* \rho k \omega \right], P_k = \mu_t \frac{\partial U_i}{\partial x_j} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (6)$$

The constants in the model are as follows: $\beta^* = 0.09$, $\alpha_1 = 5/9$, $\beta_1 = 3/40$, $\sigma_k = 0.85$, $\sigma_\omega = 0.5$, $\alpha_2 = 0.44$, $\beta_2 = 0.0828$, $\sigma_{k2} = 1$, and $\sigma_{\omega 2} = 0.856$.

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 equations for a droplet of mass m_d in the Lagrangian framework are as follows:

$$m_d \frac{dU_{i,d}}{dt} = F_{i,d} + F_{i,p} + F_{i,am} + F_{i,b} \quad (7)$$

Here, $U_{i,d}$ is the droplet velocity for i -direction and $F_{i,d}$ is the drag force, $F_{i,p}$ the pressure force, $F_{i,am}$ the virtual force and $F_{i,b}$ the body force. The definition of forces in (7) is detailed in [7].

Inserting the above mentioned various forces into (7), then the following equation can be derived

$$\frac{dU_{i,d}}{dt} = \frac{3 C_D}{4 D_d} \left(\frac{\rho}{\rho_d} \right) |U_i - U_{i,d}| (U_i - U_{i,d}) + \left(1 - \frac{\rho}{\rho_d} \right) g_i \quad (8)$$

Knowledge of the droplet velocity allows its instantaneous position vector x_i to be determined by integrating:

$$\frac{dx_{i,d}}{dt} = U_{i,d} \quad (9)$$

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. It is assumed in Kelvin-Helmholtz model that an unstable surface wave forms, grows and breaks up with the atomization length (La) and time (Ta). The primary breakup model used in this study is the Linearized Instability Sheet Atomization (LISA) model [8]. According to the model, all the injected droplets have the same diameter as that of nozzle hole and the liquid sheet velocity (V) at the injector exit, which is related to the injection pressure (Δp), is assumed to be uniform. It is given by

$$V = k_v \sqrt{\frac{2\Delta p}{\rho_l}} \quad (10)$$

where k_v is the discharge coefficient of the nozzle is given by

$$k_v = \max \left[0.7, \frac{4\dot{m}}{\pi d_o^2 \rho_l \cos \theta} \sqrt{\frac{\rho_l}{2\Delta p}} \right] \quad (11)$$

where \dot{m} and θ are the mass flow rate and spray angle, respectively, and d_o is the injector exit diameter. Once Δp is known, the axial component of the sheet velocity (u) can be found via (10):

$$u = V \cos \theta \quad (12)$$

The initial liquid sheet thickness (h_o) is obtained by mass conservation:

$$\dot{m} = \pi \rho_l u h_o (d_o - h_o) \quad (13)$$

The thickness of the liquid sheet (h), as a function of the distance from the nozzle, can be calculated assuming that V is constant in time and that the relative sheet-gas velocity is equal to the liquid near the injector.

Wave oscillation on the liquid sheet cause its breakup into ligaments and eventually the ligaments break up into droplets. The sheet will break up at a length (L) given in the original LISA model by

$$L = V \tau = 12 \frac{V}{\Omega_s} \quad (14)$$

where Ω_s is the maximum wave growth rate. If the breakup occurs when the amplitude of the unstable waves is equal to the radius of a ligament, the mean droplet diameter (D_d) is given as

$$D_d^3 = \frac{3\pi D_L^2}{K_L} \quad (15)$$

where K_L is the maximum wave number and D_L is the ligament diameter calculated from the sheet thickness at the breakup location and can be obtained from a mass balance as follows;

$$D_L = \sqrt{\frac{16h}{K_S}} \quad (16)$$

where K_S is the unstable wave number as shown in [8].

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 one of the following

modes; (1) The bag breakup, in which the non-uniform pressure field around the droplet causes it to expand in the low-pressure wake region and eventually disintegrate when surface tension forces are overcome and (2) The stripping breakup, a process in which liquid is sheared or stripped from droplet surface.

Reitz-Diwaker model has provided a criterion for the onset of break and concurrently an estimate of the stable droplet diameter, $D_{d,stable}$, and the characteristic time scale τ_b of the breakup process. The instantaneous droplet diameter is calculated as follows,

$$\frac{dD_d}{dt} = -\frac{(D_d - D_{d,stable})}{\tau_b} \quad (17)$$

The criteria and time scales for bag breakup and stripping breakup are as follows,

Bag breakup: the instability is determined by a critical value of the Webber number which is defined as,

$$We = \frac{\rho |U - U_d|^2 D_d}{2\sigma_d} \geq 6 \quad (18)$$

where U and U_d are represent the instantaneous fluid and droplet velocity, respectively, and σ_d is the surface tension coefficient. The stable droplet size ($D_{d,stable}$) is that which satisfies the equality in (18). The associated characteristic time is

$$\tau_b = \frac{\pi}{4} D_d \sqrt{\frac{\rho_d D_d}{\sigma_d}} \quad (19)$$

Stripping breakup: the criterion for the onset of the regime is

$$\frac{We}{\sqrt{Re_d}} \geq 0.5 \quad (20)$$

where Re_d is the droplet Reynolds number defined as, $Re_d = (\rho |U - U_d| D_d) / \mu$.

The characteristic time scale for this regime is

$$\tau_b = \frac{C_{s2}}{2} \sqrt{\frac{\rho_d}{\rho}} \cdot \frac{D_d}{|U - U_d|} \quad (21)$$

Here, the coefficient C_{s2} is in the range 2 to 20 [10] and the value of 20 is used in this work.

In order to reduce the NOx emissions, the technology of selective catalytic reduction (SCR) with urea is used in the present work. In the urea-SCR system, a water-urea solution (32.5 wt% urea) is sprayed into the hot exhaust stream in front of the SCR catalyst and water evaporation and thermolysis reaction of urea are occurred. The subsequent generation of NH₃ proceeds in following steps [3]; water is evaporated from a spray of UWS droplets at first. And the solid phase urea melts

at 406K and then the thermal decomposition of urea into ammonia (NH_3) and isocyanic acid ($HNCO$) momentarily [3].



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



C. 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. 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 466,199 by considering the convergence (See Fig.2).

Urea-water solution (UWS) contained solid phase urea is assumed to be a dispersed multi-phase flow so that its droplets are treated with Lagrangian particle tracking, which solves the equations of motion for parcels of droplets with adequate properties. Each particle moves randomly and collides through a unique trajectory which is formed by interaction. In addition, particles are bounced and shattered at the wall of exhaust pipe. Phenomena of heat and mass transfer and phase change cause its size to change. Therefore, in the present work, numerical analysis for the exhaust gas with high temperature is carried out first in a continuous phase and then transport phenomena of UWS using a Lagrangian framework for a dispersed phase can be obtained. In this case, a carrier stream is adopted for an exhaust gas and a computational parcels concept in which the number of particles is probabilistically occupied within the finite parcels is used for UWS. As mentioned earlier, computational simulation has carried out 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.

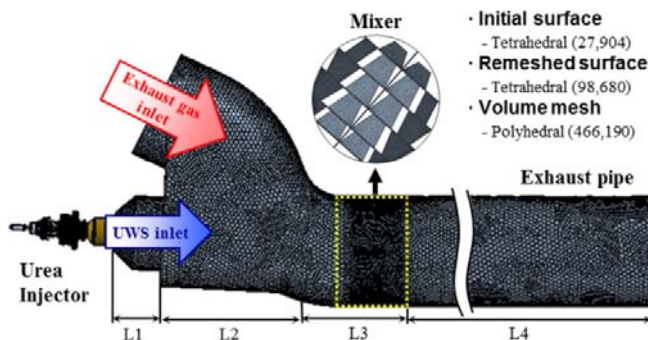


Fig. 2 Grid system for computational domain

The exhaust gas is assumed to be air because the primary objective of this study is predicted the characteristic of UWS behavior in the urea-SCR system. It enters into the system with a temperature of 300°C at a flow rate of 39.6g/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 0.262g/s. The nozzles have the same shape and size with diameter of 0.215mm. The pressure boundary condition is adopted at the exit region and no-slip boundary condition is used in all walls.

III. 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.

A. Transport Phenomena

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 chapter, 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: 0mm, the mixer is not installed)

Fig. 3 shows the average temperature and mass fractions of urea and H_2O according to the distance from the injector (x/L). The temperature has the highest value of 290°C between the exhaust gas inlet and the location of 96mm and decreases gradually toward the exit of exhaust pipe. It is due to the fact that the hot gas is mixed with a relatively cold UWS.

High performance of the urea-SCR system for the abatement of nitrogen oxides (NO_x) emission from diesel engines can be achieved from how much the total amount of NH_3 which is created by chemical reaction processes of thermolysis and hydrolysis is. In the present work, the uniformity index of NH_3 (γ , UI) which is defined in(25) is used as the performance criterion of this system. As the value of γ is closed to unit, the urea-solution is uniformly transfer to NH_3 so that the de- NO_x efficiency is improved and the slip phenomenon of NH_3 can be dramatically decreased.

$$\gamma = 1 - \frac{1}{2n} \sum_{i=1}^n \frac{\sqrt{(\omega_i - \omega_{mean})^2}}{\omega_{mean}} \quad (25)$$

where ω_i and ω_{mean} are the local and average concentration values of NH_3 , respectively, and n is the total number of measuring point.

The UI(NH_3) distributions calculated by CFD simulation according to the axial distance are shown in Fig. 4 and the mass fractions of NH_3 and $HNCO$ are also indicated for the base model. The unit value (i.e. 1.0) of UI means that the reduction

process is completed by 100%. As can be seen in Fig. 5, the UI (NH_3) is decreased until the region where exhaust gas and UWS are mixed (L_2) and then increases gradually with the maximum value of 0.78 ($x = 236\text{mm}$ or $x/L = 0.3-0.5$). Increasing in the UI is caused by the vigorous reaction of thermolysis and hydrolysis and the mass fractions of gas phase ammonia and isocyanic acid have the same trend as that of UI(NH_3) as shown in the same figure.

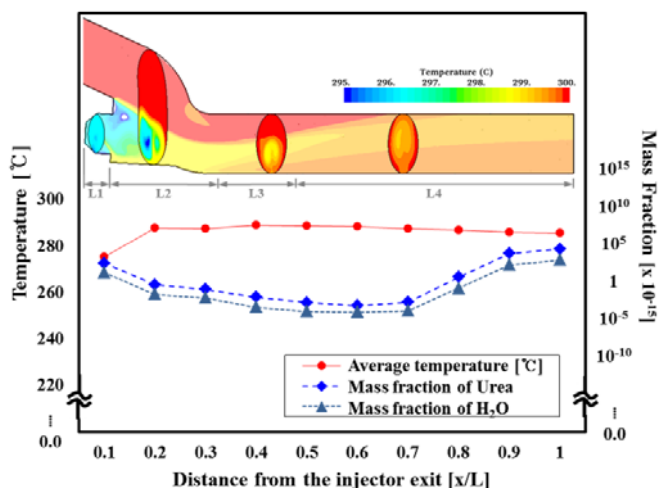


Fig. 3 Average temperature and mass fraction distribution for various locations

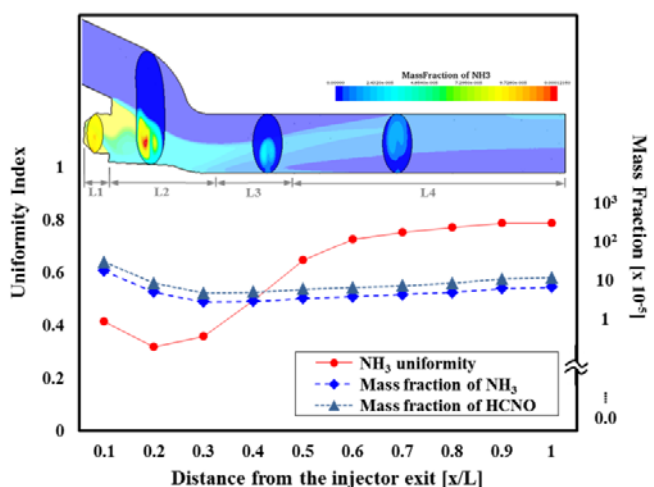


Fig. 4 Uniformity index of NH_3 and mass fraction distributions of NH_3 and HCNO for various locations

The thickness variation of fluid film according to the non-dimensional distance from the injector exit at radial direction section is presented in Fig. 5. The urea-water solution is sprayed into the hot exhaust engine gas and its behavior becomes a complex characteristic because it transforms to vapor, liquid droplet, solid urea, gas phase NH_3 , and HNCN. As indicated this figure, the wall-wetting is initially occurred at the position of 125mm in the exhaust pipe and the constant pattern is repeatedly appeared because of the pulsating motion by a vortex. From the point of physical concept, the occurrence of

the wall-wetting is due to the following fact; small droplets, which are created both by the mass reduction and collision with wall, generally flows out with the exhaust gas. On the contrary, the bigger droplets can be generated by the mass accumulation and deposition by collision and restraint a vaporization process because they collide with wall and decrease the exhaust gas temperature. This phenomenon is a primary reason for wall-wetting occurrence. Therefore, for minimizing the wall-wetting the injection angle (or direction) of the urea injector has to be adjusted through the design optimization. This result also gives very interesting information for the installation location of mixer.

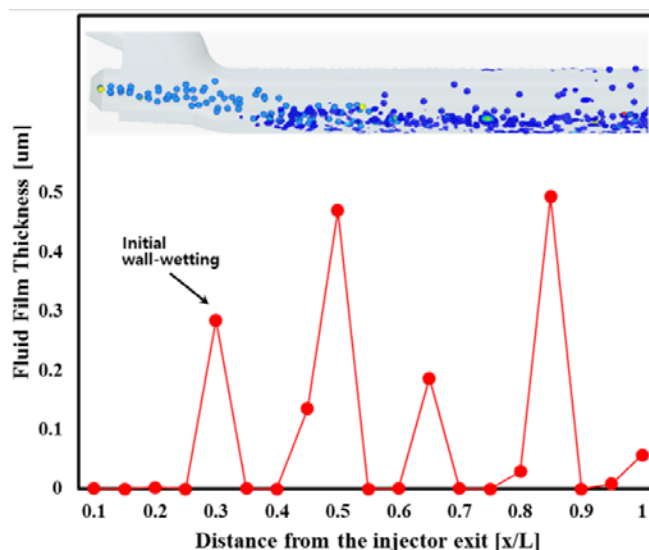


Fig. 5 Total thickness of fluid film for radial-axis section

B. Effect of Mixer

In this section, the influence of the mixer on the transport phenomena is examined through the flow and chemical reaction characteristics and the UI (NH_3). As discussed in Fig.5, in the present work, the mixer is installed at the position of 130mm 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.6. It can be seen in the figure 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 with mixer, the high pressure field 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. It causes the velocity to increase from 7.25m/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 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, as shown in Fig. 6. 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.

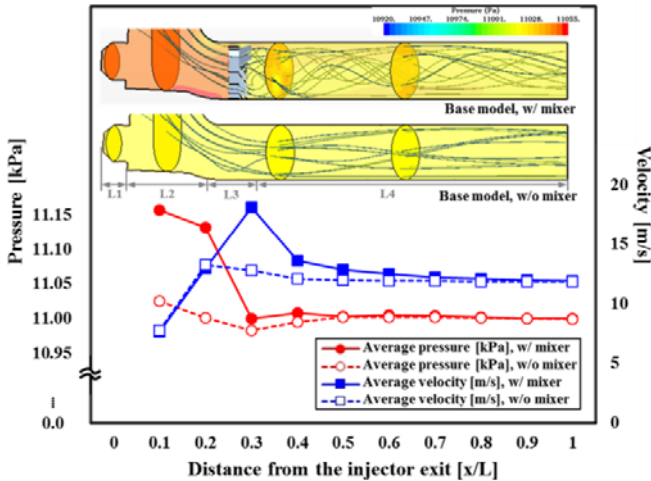


Fig. 6 Flow characteristics for the cases of w/ and without mixer

Fig. 7 shows the distribution of uniformity index of NH_3 (UI) 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). As shown in Fig. 7, it looks like almost same trend until at $L = 150\text{mm}$ from the injector irrespective of the existence of mixer. The $\text{UI}(\text{NH}_3)$, however, is increased abruptly after the mixer. Therefore, the $\text{UI}(\text{NH}_3)$ for the case of with mixer is increased by 17.95% compared to that of without mixer (that is, the value of $\text{UI}(\text{NH}_3)$ 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 hydrolysis and thermolysis in the exhaust pipe. It is also found from the result that the NO_x emission effect is increased when the mixer is installed in the exhaust pipe qualitatively. This considerable alteration of flow field causes to the increasing the mass fractions of NH_3 and HCNO , as presented in Fig. 8.

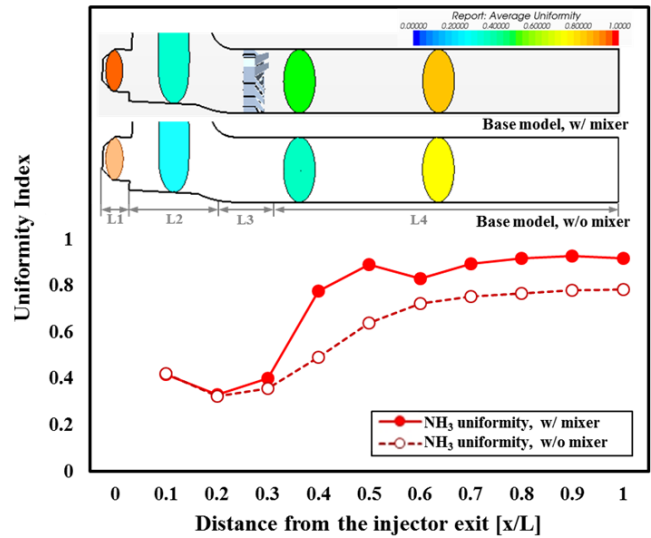


Fig. 7 Uniformity index (UI) of NH_3 for the cases of w/ and without mixer

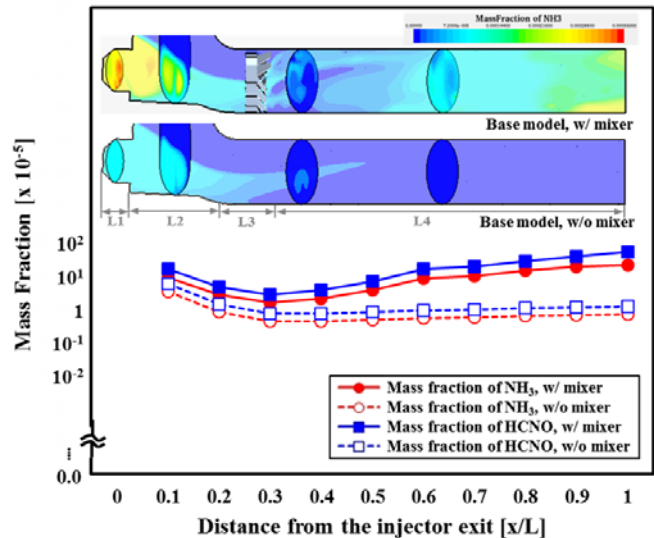


Fig. 8 Mass fractions of NH_3 and HCNO for the cases of w/ and without mixer

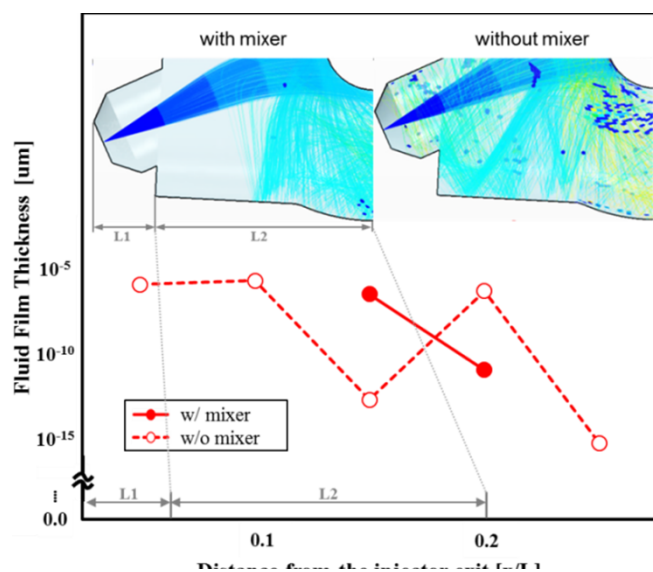


Fig. 9 Film thickness for the cases of w/ and without mixer

In the practical point of view, a solid state urea may give rise to the blockage of the nozzle and it is need to minimize the accumulation of UWS on the wall. Therefore, in the present study, the concept of fluid film thickness is introduced in order to investigate the influence of the mixer on the wall-wetting and its distributions and average values for some positions are shown in Fig. 9. It can be seen in the figure that the fluid film thickness for the case of with mixer is predicted as 98% lower value compared to that of without mixer. From the results the existence of mixer causes the improving the performance of urea-SCR system by increasing the efficiency of catalyst reduction as well as the preventing the nozzle blockage by minimization of accumulation of solid-state urea.

IV. 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 pipe 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), respectively.

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Kyungwoo Park was born in Seoul, Korea in February of 1961. He has received his BA degree in 1985, MA degree in 1990, and Ph.D. degree in 1995, respectively, at the department of mechanical engineering of Hanyang University, Seoul, Korea. He is currently working at Department of Mechanical Engineering in Hoseo University as a professor. As soon as he acquired his Ph.D. degree, he entered the LG Industrial Systems Co., Ltd., and he researched on the flow and thermal characteristics around/in elevators. His main interesting fields are heat transfer, micro/macro thermo/fluid dynamics, optimization, and CFD. Recently, his researches are focus on the semiconductor and display manufacturing process and the aerodynamics and optimization of fluid/thermal systems.