

Article

Investigation of Solid Deposit Inside L-Type Urea Injector and NO_x Conversion in A Heavy-Duty Diesel Engine

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Abstract: The heavy-duty diesel engine is used in the main transportation vehicles in Korea to deliver products from various companies; however, diesel engines produce enormous quantities of nitrogen oxide (NO_x), which harms human health. The selective catalytic reduction (SCR) system is a common solution to reduce NO_x emissions from diesel engines; however, heavy-duty diesel engines produce more NO_x than can be dealt with using an SCR and thus require investigations into effective NO_x reduction solutions. This study investigated 12,000 cc heavy-duty diesel engines from Hyundai using the 1000 rpm engine operation to produce 1330 ppm of NO_x emission. The ammonia generation process was assessed by the amount of ammonia produced; the amount of ammonia gas was identified by 19 gas sensors on the catalyst surface; the effectiveness of the mixing process between the ammonia and the NO_x in the system was determined by the NO_x conversion values from a gas analyzer. Comparison between the experiment and simulation results shows the ammonia and NO_x values and elucidates the temperature results for vaporization and saturation quantity, ammonia distribution, and NO_x conversion in the system. The NO_x conversion investigations also provide the chemical reaction and numerical equation relevant to the ammonia and NO_x distribution.

Keywords: kinetic modeling; injection pressure; ammonia gas; NO_x storage reduction; particulate filters

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1. Introduction

Since the increasing individual mobility of on-road and off-road transportation in the 20th century, human-made vehicles, such as cars, trucks, buses, etc., produce significant emissions, which can damage the human body from the inside. The current automotive industry can control otto engine emissions by three-way catalytic converters, but that solution cannot solve the diesel engine problem [1]. The Korean government regulation limits are strict to reduce nitrogen oxide (NO_x) emissions from transportation engines because every year, the number of vehicle users always increases, resulting in more emissions [2]. The diesel engine is in great demand, being used in public transportation and freight carriers, but these engines can produce more NO_x emissions than other types of engines. Accordingly, the automotive industry is trying to improve diesel engines to comply with government regulations [3]. One approach is selective catalytic reduction (SCR) systems, which can produce ammonia particles to control NO_x emissions from diesel engines.

Briefly, the SCR process to reduce NO_x emissions from an engine is as follows: (1) a urea–water solution (UWS; AdBlue) is injected into the SCR system as small droplet particles; (2) the urea droplet will breakup after hitting the wall system; (3) the small urea

droplets evaporate, becoming ammonia gas due to the hot gas temperature; (4) the ammonia gas then mixes with the NO_x emission gas, which produces nitrogen (N_2) and steam (H_2O) in the system. This process and reaction can reduce NO_x emissions from diesel engines. However, this process is usually not as smooth as the theory; many factors create difficulties in mixing ammonia with the NO_x emission. The urea particles often get stuck in the injector and cannot spread through the system [2]; the injector often struggles to spray urea in small droplets [4]; the large urea particles from the injector easily attach to the system [5]; the exhaust temperature and wall temperature (T_w) make it difficult to evaporate the urea droplet [6], which produces solid deposit formations in the system [7].

Many researchers have modified SCR systems to improve the output, such as by changing the injector position to improve the spray phenomena [8]; adding a mixer fan to increase the distribution flow inside the system [9]; raising the wall temperature to increase the evaporation process [10]; using different injector models to inject the urea. This research has improved SCR system performance to decrease the NO_x quantity from diesel engines; however, every engine different challenges. The urea evaporation model for small engines is difficult to apply to larger engines. Khristamto [2] studied the ammonia uniformity with two injector models, focusing only on the ammonia production and ammonia homogenization on the catalyst surface; however, this does not clearly explain the SCR system problem. To address this issue, in this study, we investigated the inside phenomena not explained in the previous study and detail the NO_x conversion in a heavy-duty diesel engine.

The 12,000cc diesel engine from Hyundai that produces 1330 ppm NO_x concentration in 1000 rpm was investigated in this study. The amount of ammonia gas influences the mixture process in the system; when the amount of ammonia gas is lower than the NO_x emission gas, the mixture between the gases will not be balanced, which can affect the removal of the NO_x emission gas from an SCR system. Computational fluid dynamics (CFD) were used to identify the flow reaction and distribution inside the system [5].

2. Result and Discussion

2.1. Urea Injector Phenomena

The urea injector is the main tool in the SCR system. The urea injector injects the urea water solution (UWS) into the system to produce ammonia gas. The Hyundai D6CC is the commercial SCR system used in this study. The original urea injector model was explained by Khristamto [2]. Figure 1 shows the original urea injector from the Hyundai D6CC and demonstrates how a specific part was hampering the gas flow. The original urea injector from the Hyundai D6CC has three spray holes with a 120 μm hole diameter, and each hole can produce a high urea mass flow rate of 8.05×10^{-5} kg per second. The UWS is easily affected by high temperatures, and as a result, solidifies; Koebel et al. [11] explained the thermal temperature and urea hydrolytic decomposition process that occurred in the 150 $^\circ\text{C}$ to 500 $^\circ\text{C}$ temperature range.

Figure 2 shows the solid urea deposit inside the original urea injector of the Hyundai D6CC. The investigation by the micro camera can show the solid deposit in the nozzle of the injector. These solid deposits lessened the distribution of urea into the system. Khristamto [2] showed the differences in ammonia quantity between the original urea injector of the Hyundai D6CC and the suggested urea injector.

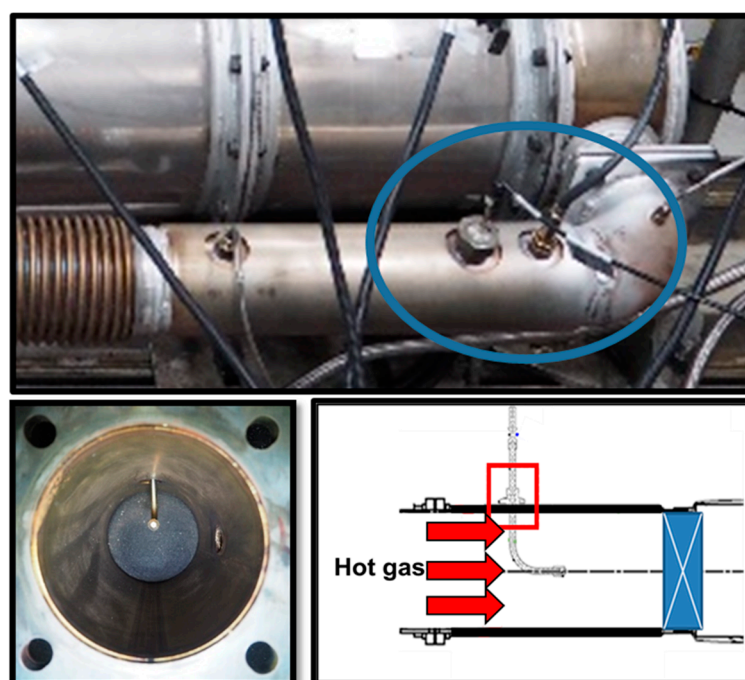


Figure 1. The original urea injector from Hyundai D6CC diesel engine.

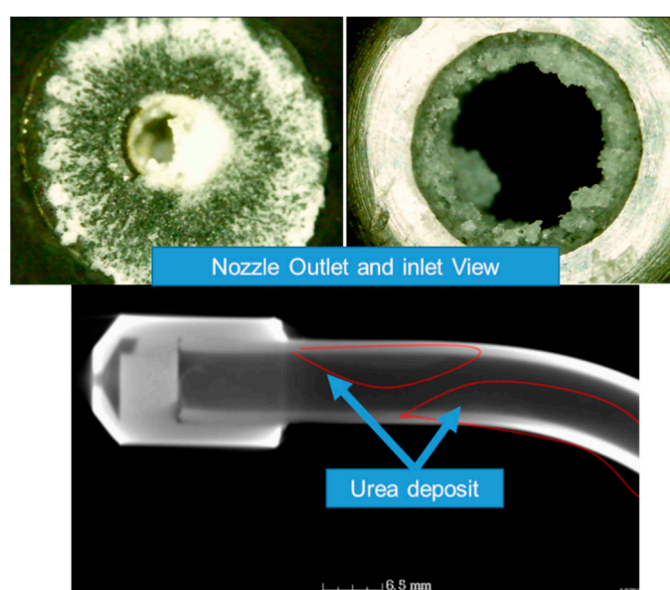


Figure 2. The solid deposit formation inside the original urea injector from the Hyundai D6CC diesel engine.

2.2. UWS Saturation and Vaporization Processes

A simulation study is a useful way of investigating phenomena that are difficult to show experimentally, especially inside a commercial SCR system from a Hyundai D6CC. Figure 3 shows the simulated urea saturation phenomena in the system; the saturation pressure from the suggested urea injector for the Hyundai D6CC obtained a higher value for producing ammonia gas in the system; this result is also found by Khristamto [2], who investigated temperature phenomena in their study. The engine exhaust temperature and gas flow were the most important indicators that assist ammonia gas generation. The UWS has 60% water (H_2O) and 40% urea; investigating the H_2O and urea saturation values allows predicting the ammonia generation process. This investigation also showed a higher concentration near the SCR catalyst, revealing that the area nearer to the catalyst has a

higher gas pressure concentration. The catalyst surface had small pores (less than 50 nm), making it an efficient filter for producing a low NO_x concentration value. The high-pressure concentration near the catalyst also assists the mixing process between the ammonia gas and the NO_x emission in the system. Figure 4 shows the urea vaporization values from the original urea injector and suggested urea injector; the exhaust gas temperature from heavy-duty diesel engine assisted the vaporization value result. In this study, the 1000 rpm engine operation produced 686 K of heat to assist the saturation and vaporizing process. In an experiment with a commercial SCR system, the urea injector would spray the urea liquid, allowing researchers to see the solid deposit phenomena occurring on the wall of the system. The solid deposit informs us of the change in quality from urea to ammonia in the system; however, the solid deposit phenomena are difficult to demonstrate in the simulation. The saturation and vaporization values can reveal the change in quality from urea to ammonia without directly seeing solid deposit phenomena in the system.

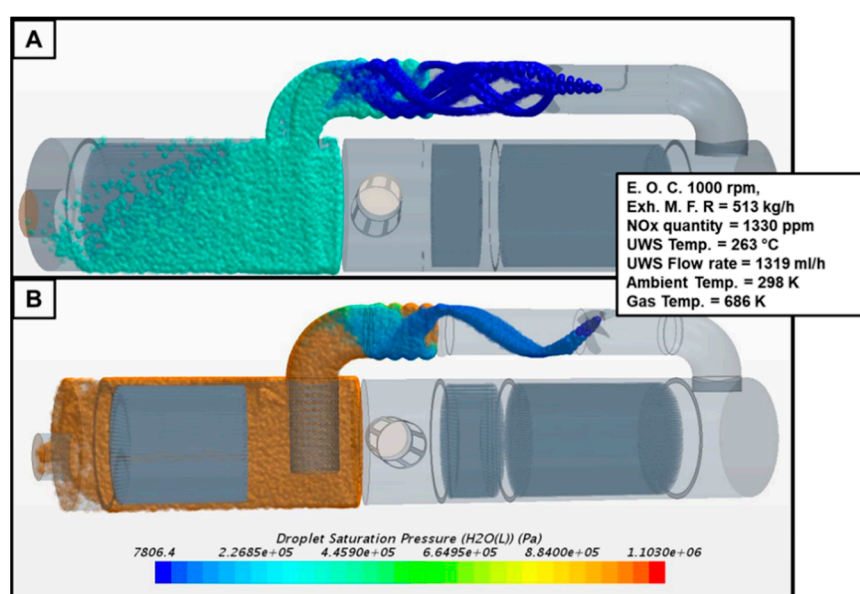


Figure 3. The urea saturation value: (A) original urea injector; (B) suggested urea injector for Hyundai D6CC.

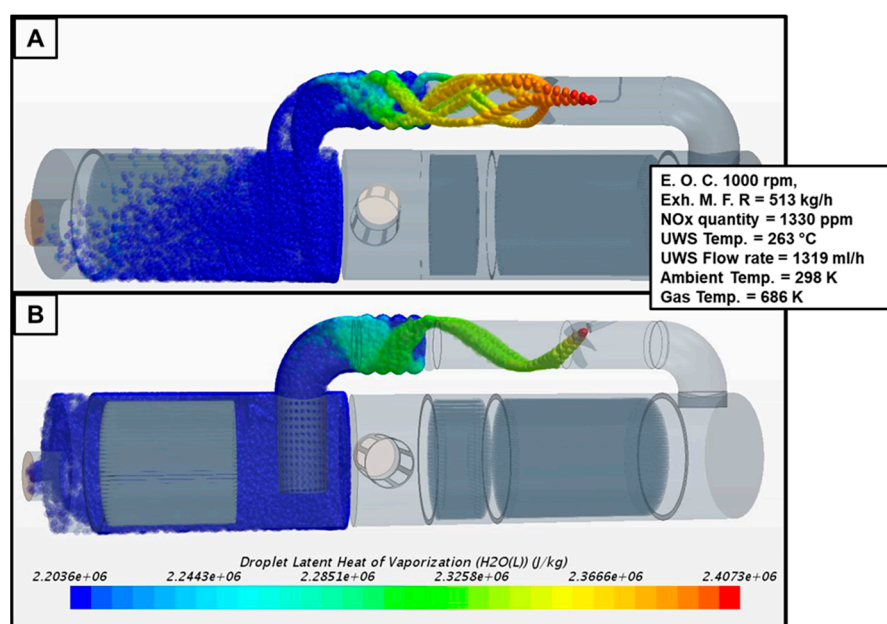


Figure 4. The urea vaporization values: (A) original urea injector; (B) suggested urea injector for Hyundai D6CC.

The velocity pattern from the simulation elucidated the gas distribution in the system. As shown in Figure 5, the UWS was easily distributed within the system, and the velocity pattern was aligned with the saturation and vaporization results from Figures 3 and 4. The distribution gas can assist in predicting the process of generating ammonia gas in the system. Based on the velocity value, the saturation and vaporization results demonstrate high values near the injector inlet; this also shows higher ammonia generation in that position, making it possible to develop a strategy to increase the reduction of NO_x emissions from diesel engines. The simulation parameters were based on experiments with an actual engine, so the simulation results and phenomena also occurred inside the experimental system.

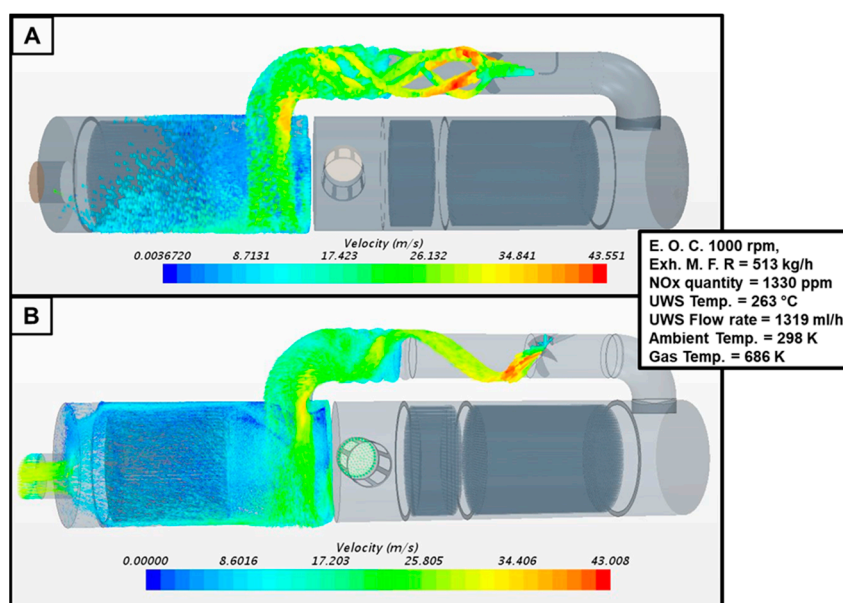


Figure 5. The pattern value of urea: (A) original urea injector; (B) suggested urea injector for Hyundai D6CC.

The urea distribution in the system can be affected by the exhaust gas. The Hyundai D6CC heavy-duty diesel engine produced a large exhaust mass flow rate (513 kg/h) and NO_x flow rate (1083 g/h). Those gas flow rates were assisted the UWS distribution to the entire system. In this section, we discuss and demonstrate the UWS distribution and explain the efficiency of the ammonia generation process, as seen in Figures 3 and 4.

2.3. The Ammonia Distribution and NO_x Conversion Value

In the gas distribution described in the previous section (UWS saturation and vaporization processes), the suggested urea injector was demonstrated to produce more ammonia than the original urea injector; the vaporization and saturation processes performed better with the suggested urea injector. Figure 6 shows the various gases in the SCR system based on time duration. This simulation study used five gas parameters—H₂O, N₂, CO₂, NH₃, and O₂—to represent the (NH₂)₂CO used in the experimental system. The transformation of the chemical form cannot be displayed in the simulation with STAR-CCM+ but can be described by describing the chemical properties formed by the chemical process. Figure 6 explains the various gases inside the system used in the general reactions that occur for urea in the SCR system. Reaction (1) is the thermolysis of urea; this process describes when NH₃ reacts with NO_x emission; reaction (2) is an isocyanic acid hydrolysis

reaction to produce the NH_3 by HNCO ; reactions (3) are standard SCR reactions to demonstrating that the NO_x emission converted to N_2 and H_2O .

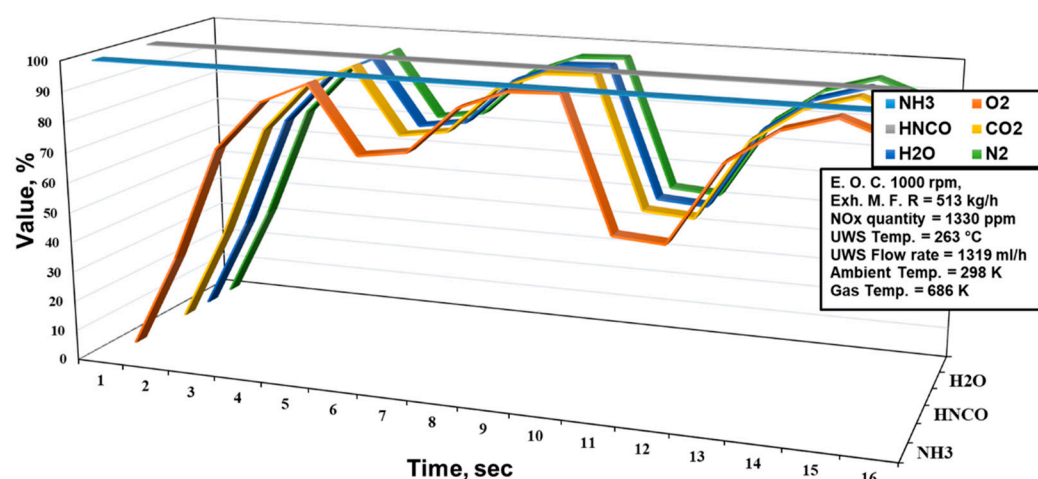


Figure 6. Various gases in the system.

Figure 7 shows the 19 sensors on the catalyst surface and Figure 8 shows the ammonia concentration value from the gas analyzer. The results show that the suggested urea injector for the Hyundai D6CC (blue bars) produced more ammonia than the original urea injector from Hyundai D6CC (red bars); more ammonia in an SCR system is also indicative of higher NO_x conversion. Figure 9 compares the amounts of NO_x conversion from the experiment. The suggested urea injector converted more NO_x than the original urea injector. This result shows that the suggested urea injector has a suitable shape and position for urea injection in a commercial SCR system by Hyundai D6CC, enhancing the urea particle conversion into ammonia and minimizing the possibility of solid deposits inside the injector. Therefore, this urea injector is recommended to improve NO_x conversion in Hyundai D6CC and can be used for other commercial SCR systems that use different types of heavy-duty diesel engines.



Figure 7. Sampled ammonia values in the catalyst inlet.

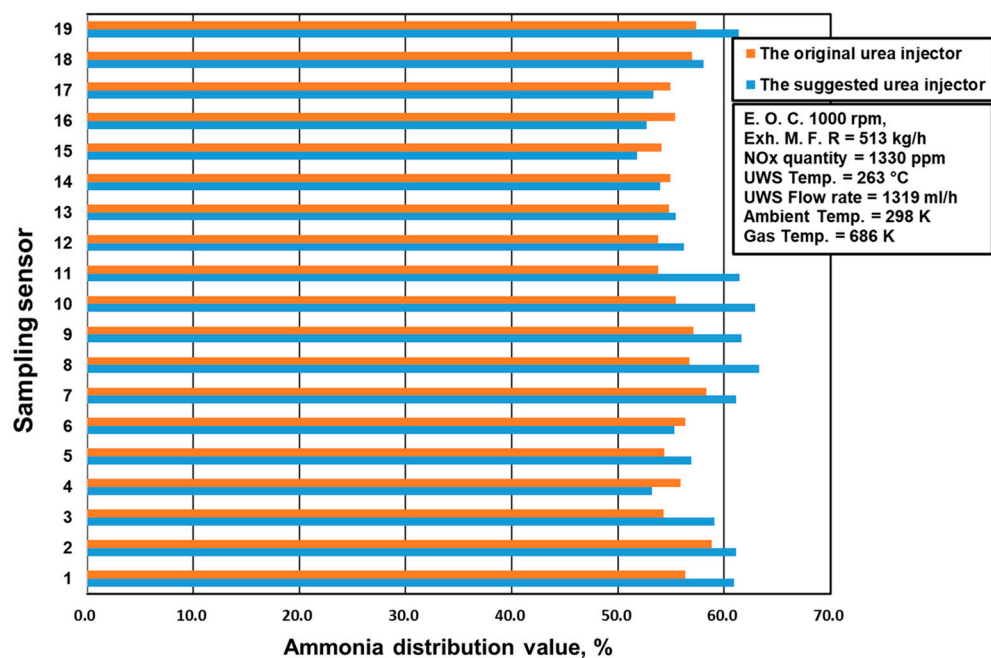


Figure 8. Sampled ammonia values by the 19 sensors in the catalyst inlet.

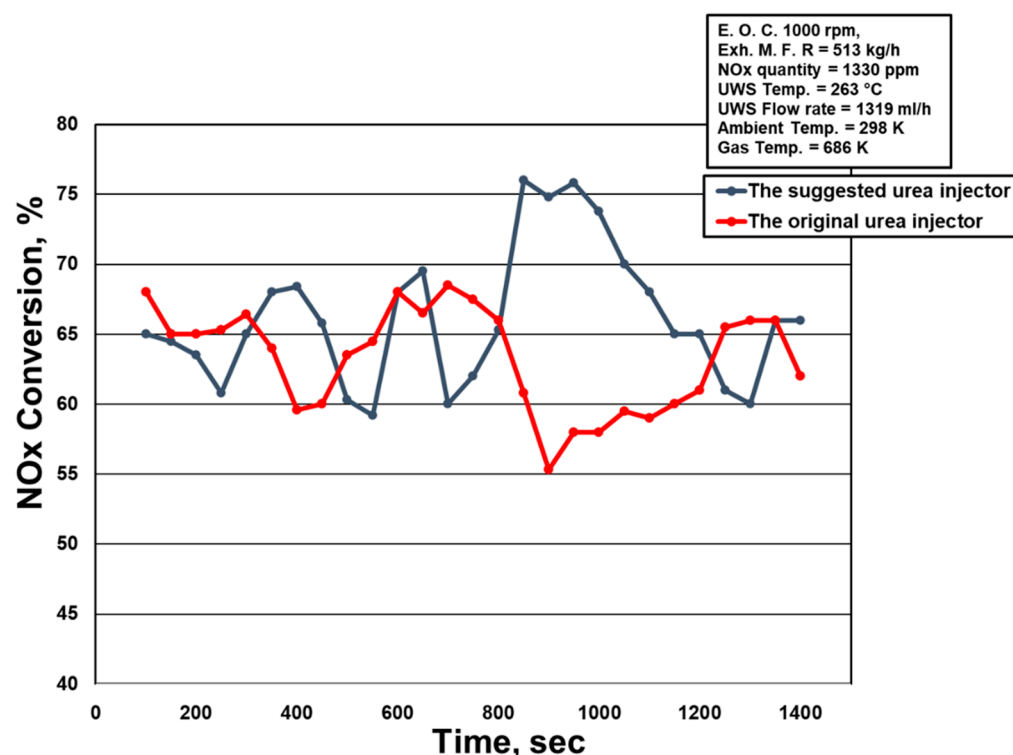


Figure 9. NOx conversion value by MEXA-7100 gas analyzer.

3. The CFD Model and The Parameter Condition

The three-dimensional (3D) CFD model is useful to observe urea injection shaping, gas distribution, ammonia patterns, and temperature values in an SCR system. This simulation study used a 3D model of CFD results to clearly show the flow distribution, temperature value, and other information. This information shows the flow pattern using color values, graphics, and other information from the simulation [5].

Turbulence simulation is an interesting way to investigate SCR systems. Yi [9] made some interesting discoveries in turbulence models in SCR systems while analyzing the effects of different mixers to optimize ammonia uniformity. In their simulations, Yi used Navier–Stokes equations renormalized by RNG for k-epsilon turbulence models. The UWS was injected from the top at a 90° angle to the system, and the urea particle droplets were released to the main flow and directly hit the wall in the system. A mixer was used to increase the flow quantity in the system. Based on the simulation, they were able to investigate the mixer fan effect on ammonia uniformity.

Khristamto et al. [6] used two CFD models; various CFD models can detail the NOx conversion in an SCR system. In the first CFD model, the UWS was injected from the top with a 90° angle and 10 cm from the inlet catalyst; the urea was injected directly into the gas flow of the SCR system. The CFD result clearly showed the UWS decomposition process and gas temperature in the SCR system; the other CFD model used was sourced from a Mercedes Benz ML350 (commercial SCR system). The urea was injected from the top of the system at a 15° angle. Based on that simulation, they could predict the gas quantity and the effect of temperature to increase the decomposition process for urea in the SCR system.

The CFD model from the D6CC commercial SCR system is shown in Figure 10. The first CFD model used an original urea injector, while the second CFD model used the suggested urea injector [2]. Various urea injectors were analyzed for the ammonia generation process and NOx conversion value. The SCR catalyst used for this study was vanadium-catalyzed; this catalyst material can support oxidative C–C and C–O bond cleavage,

carbon–carbon bond formation, deoxy-dehydration, hydrogenation, and dehydrogenation [12].

Figure 11 shows the model and shape of two urea injectors in this study with the same holes and urea value parameters [2]. The simulation parameters were used in this study based on the experiment study with Hyundai D6CC. Thus, the dimensions and size of the SCR system matched the actual system. That varies of urea injector had a height of 152 mm, 6.5 mm diameter, and three spray holes with a 120 μm hole diameter. Each hole can produce a high urea mass flow rate of 8.05×10^{-5} kg per second.

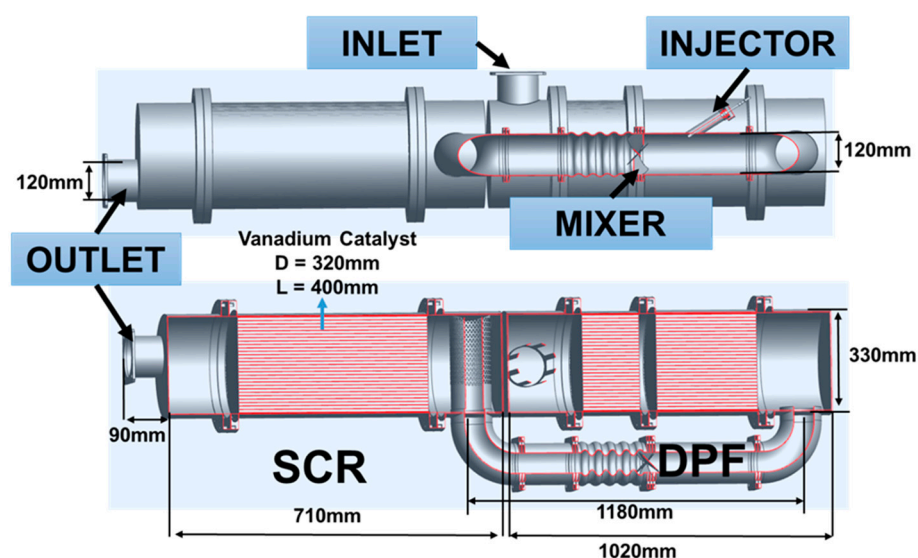


Figure 10. The CFD model for the SCR system (D6CC by Hyundai) [2].

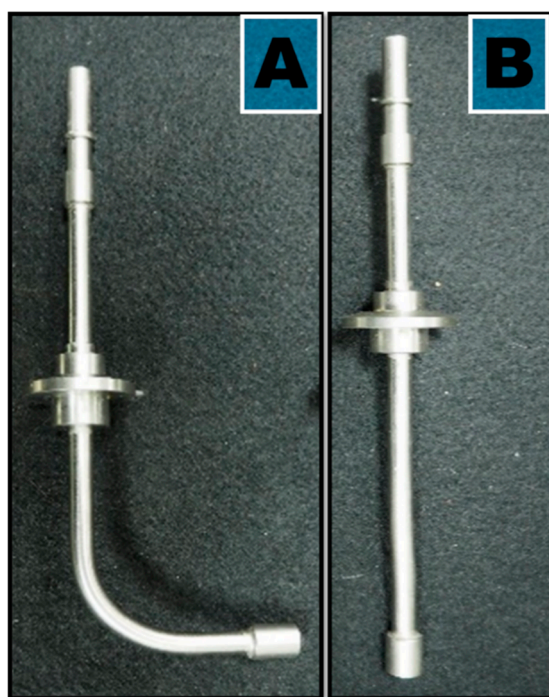


Figure 11. The two urea injector models: (A) the original injector from the D6CC diesel engine; (B) the suggested urea injector [2].

In the CFD study from Fischer et al. [13], the simulation equation of the Reynolds stress model was adopted for computing the anisotropic characteristics since that method

can investigate the turbulence phenomena in the swirl flow. In this current study, a mixer fan was used to increase the flow distribution and assist the chemical reaction between the ammonia and NO_x in the system. A simulation with the Reynolds-Averaged Navier–Stokes (RANS) equation can analyze the flow characteristics and flow distribution. The gas flow in this simulation is described with the turbulence equation, which is visualized by the flow distribution pattern. The RANS modeling was useful to increase the turbulence kinetic energy (TKE) quantity in the SCR system cross-sections, given the relatively low dissipation in the swirl flow.

A polyhedral mesher with three prism layers and a 10 mm mesh size was used in this simulation study; this method can show scalability and mesh quality. The meshing scale for polyhedral can observed more than 60m core cell on 250+ cores; this meshing result can produce a smoother surface in this study. The velocity vectors formed a vector field, which was assumed as the transport equations for the RANS model and solved the computational domain. The equation for eddy viscosity modeling assumed the isotropic turbulence value, and the TKE (k) followed the Reynolds stress modeling equation:

$$k = \sum_{i=1}^3 \frac{\overline{U_i^2 U_i^2}}{2}. \quad (4)$$

The RANS model can compute the complete tensor in the equation. The components from the RANS model can be directly inserted into the flow measurement system. Equation (5) and Equation (6) inform the calculation for turbulence intensity $\overline{U_i^2 U_i^2}$ to investigate the flow velocity value (u) on the i -direction:

$$\overline{u_i} = \frac{1}{N} \sum_k u_{k,i} \quad (5)$$

$$\overline{U_i^2 U_i^2} = \frac{1}{N} \sum_k (U_{k,i}^2 - \overline{u_i}^2). \quad (6)$$

The quasi-steady evaporation model in this simulation allowed the urea droplet particles to lose mass. The driving force in the evaporation and condensation process can maintain the equilibrium of the liquid–vapor system. The UWS used in this study had 60% water and 40% urea [14]. The wall temperature assists the urea particle to evaporate; the heat transfer equation calculates the evaporation rate, thereby ensuring the saturation temperature can vapor the urea particle.

$$\sum_i X_{is} \geq 1 \quad (7)$$

where X_{is} is the equilibrium mole fraction of transferred the component for urea particle; the Raoult's law method is used to find the value of X_{is} :

$$X_{is} = \frac{p_{sat}^i(T_p)}{p} X_{ip} \quad (8)$$

where $p_{sat}^i(T_p)$ is the component saturation pressure that is evaluated at the wall temperature in the SCS system, and X_{ip} is the component mole fraction in the urea droplet particle; when the condition in Equation (7) is satisfied, the urea particle vaporize in proportion to their mass fractions. The range urea particle diameter in this simulation used the Rosin–Rammler particle size distribution; this method size distribution is a smooth continuous distribution depending on four parameters: reference size, exponent, minimum size, and maximum size. The exponent was developed to describe the volume distribution of urea particles as a function of their diameter as follows:

$$F(D) = 1 - \exp \left[- \left(\frac{D}{D_{ref}} \right)^q \right] \quad (9)$$

The particle size was quantified using a cumulative distribution function, which is $F(D)$. The mass parameters are the exponent q , the Rosin–Rammler diameter is D_{ref} and the urea particle size D ; this form confirmed that the Rosin–Rammler particle size could investigate the urea distribution value based on the cumulative mass, volume, or number

distribution, depending on the flow rate specification of the urea injector. When the condition in Equation (6) is satisfied, the volatile components in proportion mass fractions, that is:

$$\varepsilon_i = \frac{Y_{ip}}{\sum_T Y_{ip}} \quad (10)$$

where the second condition for a saturated vapor is:

$$\sum_T Y_i = 1 \quad (11)$$

where Y_{ip} is the mass fraction of component “i” with the pressure value and Y_i is the mass fraction of component of “i” with free stream value; that equation is the cell containing the urea droplet particle; the index “i” refers to the mixture of gaseous components; ε_i is the fractional mass transfer; $\sum_T$ is the temperature transfer components. Effectively, the transfer number represents the driving force for evaporation, which is a function of thermodynamic conditions for the liquid and vapor. Conductance, on the other hand, represents geometrical and mechanical effects, such as the urea droplet size and velocity distribution. However, the transfer number for saturation vapor can be described with:

$$B = \frac{c_p (T - T_p)}{\sum_T \varepsilon_i L_i} \quad (12)$$

where B is the Spalding transfer number for heat transfer; T is the temperature; T_p is the particle temperature; c_p is the gas specific heat; L_i is the latent heat component. The urea saturation process will produce ammonia gas and will mix in the system; based on that condition, the multi-component equation gas was used in this study, as follows:

$$\frac{\delta \rho_j a_j Y_{j,i}}{\delta t} + \nabla \cdot (\rho_j a_j Y_{j,i} v_j) = \nabla \cdot (\rho_j a_j D_j \nabla Y_{j,i}) + S_{j,i} + \dot{m}_{j,i} \quad (13)$$

where ρ_j , a_j , and v_j are the density, volume fraction, and velocity of phase j, respectively; $Y_{j,i}$ is the mass fraction of species i in phase j, that is, the fraction of the total mass of that phase; D_j are the mass diffusivity numbers with the combining the molecular particle and gas turbulent in the system; $S_{j,i}$ is a general mass source; $\dot{m}_{j,i}$ is used here to refer specifically to the transfer of species from one phase to another if there is a single phase with a_j equal to 1 and no interphase mass transfer in the system. The NO_x conversion value for an SCR system is shown in Equation (14), where the NO_x gas quantity after the SCR system divides the NO_x gas emission from the engine:

$$NOx_{conversion\ value} = \left(1 - \frac{NOx\ Outlet}{NOx\ inlet}\right) \times 100\% \quad (14)$$

4. The Experimental Model and the Parameter Conditions

These experimental studies used a six-cylinder four-stroke heavy-duty diesel engine and water-cooled with natural aspiration. The 1000 rpm engine speed produces a 513 kg/h exhaust mass flow rate and a 1330 ppm NO_x value with NO₂/NO_x feed ratio (0–1) and keeps the NH₃/NO_x feed ratio alpha=1 [6]. The Hyundai D6CC diesel engine produces a high NO_x emission at 1000 rpm and is easy to observe in the system. The exhaust gas concentration was computed using the gas analyzer before the experimental study. The uncertainty of coefficients exhaust gas from the gas analyzer (MEXA-7100 DEGR; Horiba ATS, Kyoto, Japan) was 5% or 1.0 µm uncertainty [15]. The experimental setup and schematic diagram of the current study are shown in Figure 12.

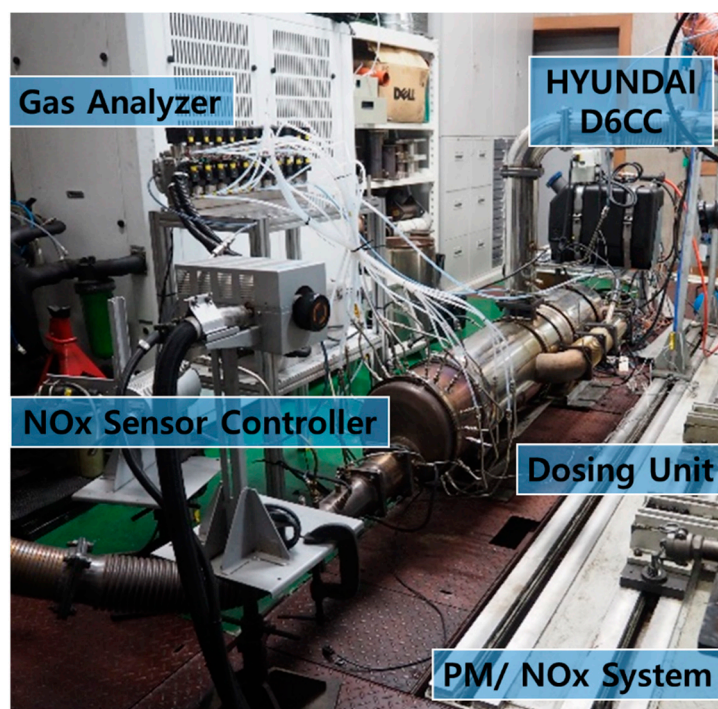


Figure 12. Experimental test and engine measurement setup.

The UWS has a 1319 ml/h urea flow rate and a 298K ambient temperature (T_g), injected into the system with an engine exhaust temperature of 686K [16]. The mixing process between NO_x emission and ammonia gas occurred from the urea injector to the catalyst surface. The outlet pipe after the SCR process connects to a gas analyzer; this analyzer informed us of the concentration value of NO_x emissions, which showed the comparative effectiveness of the original urea injector and the suggested urea injector in the system. The sampling for that experiment was repeated 10 consecutive times.

5. Conclusions

The investigation of solid deposits made inside the urea injector and NO_x conversion in a heavy-duty diesel engine revealed a phenomenon that was hidden from the previous result by Khristamto [2]. The study with a 12,000cc heavy-duty diesel engine in 1000 rpm operation produced a 513 kg/h exhaust mass flow rate, a 1330 ppm NO_x value, and a 686 K exhaust gas temperature. The original urea injector shows the compaction of urea inside the injector, thus inhibiting the urea injection process. This phenomenon has a negative effect on the NO_x conversion efficiency in a Hyundai D6CC. Based on that problem, the suggested urea injector, as shown in the previous result by Khristamto [2], was used to solve the solidification of urea inside the injector, as the shape and position of the injector were suitable for the SCR system. The suggested urea injector can produce a larger ammonia amount by its excellent urea saturation and vaporization results.

The ammonia gas amount is the main indicator to improve NO_x conversion in the system. The chemical reaction to demonstrate NO_x emission converted to N_2 and H_2O , requires an equal amount of ammonia gas; the system should produce enough ammonia gas to solve that situation. The suggested urea injector can improve the amount of ammonia gas, which was demonstrated by our experiments using 19 gas sensors in the catalyst surface and a gas analyzer. The NO_x conversion value in these results can validate the ammonia amount from the suggested urea injector and complement the previous study by Khristamto [2]; these results imply this urea injector is applicable for use in heavy-duty diesel engines, specifically the Hyundai D6CC. Thus, this study is a good reference for future research into decreasing NO_x emissions from heavy-duty diesel engines, especially engines with similar parameters.

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Conflicts of Interest: The authors declare no conflict of interest.

Nomenclature

RANS	Reynolds Average Navier Stokes
CFD	Computational Fluid Dynamics
UWS	Urea Water Solution
SCR	Selective Catalyst Reduction
H ₂ O	Hydrogen
NO _x	Nitrogen Oxide
N ₂	Nitrogen
O ₂	Oxygen
K	Kelvin temperature
UI	Uniformity Index
TKE	Turbulent kinetic energy (k)
RNG	Renormalization group
DPF	Diesel Particulate Filter
PM	Particular meter
NH ₃	Ammonia gas

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