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Chien NGUYEN HUY¹, Tuyen PHAM HUU², Thanh DINH XUAN³

SIMULATION TO DETERMINE THE APPROPRIATE UREA INJECTION ANGLE IN A SELECTIVE CATALYTIC REDUCTION SYSTEM

Summary. The selective catalytic reduction (SCR) system is the most effective approach to reducing nitrogen oxide (NO_x) emissions in diesel engine exhaust gases. The NO_x conversion efficiency of SCR systems depends on several factors, including exhaust gas temperature, urea injection and evaporation characteristics, NH₃/NO_x distribution uniformity, exhaust gas flow rate, and urea consumption. This paper evaluates the effect of urea injection angle (β) on the wall spray behavior, the exhaust gas temperature, and gas mixture uniformity at the inlet of the SCR catalyst. The study used ANSYS Fluent CFD (computational fluid dynamics) simulation software with angles $\beta = 20^\circ, 30^\circ, 45^\circ, 90^\circ$, and 135° . The research results show that urea injection angles $\beta = 20^\circ$ and 30° reduce the amount of urea solution sprayed and adhered to the exhaust pipe wall. The gas mixture temperature distribution at the SCR catalyst inlet ranges from 444.28 K to 677.21 K, which corresponds to the effective operating temperature range of the SCR catalyst. At a urea injection angle of $\beta = 30^\circ$ at the SCR catalyst inlet,

¹ School of Mechanical Engineering, Hanoi University of Science and Technology, No.1 Dai Co Viet, Bach Mai, Hanoi, Vietnam. Email: chiennh@hau.edu.vn. ORCID: <https://orcid.org/0000-0002-0919-1865>

² School of Mechanical Engineering, Hanoi University of Science and Technology, No.1 Dai Co Viet, Bach Mai, Hanoi, Vietnam. Email: tuyen.phamhuu@hust.edu.vn. ORCID: <https://orcid.org/0000-0002-5401-2643>

³ School of Mechanical and Automotive Engineering, Hanoi University of Industry, No. 298 Cau Dien Street, Tay Tuu Ward, Hanoi, Vietnam. Email: thanhdh@hau.edu.vn. ORCID: <https://orcid.org/0000-0002-5262-4443>

the NH_3 /gas mixture is mixed most uniformly ($\text{UI} = 0.826$) at an engine rotation of 2000 rpm and a load of 100%.

Keywords: urea injection angle, SCR technology, NO_x emission reduction, diesel engine, engine exhaust gases

1. INTRODUCTION

In the SCR system, a urea solution is injected into the heated engine exhaust gas, where it is hydrolyzed to ammonia (NH_3), which serves as a reducing agent, reacting with NO_x to form N_2 and H_2O on the catalyst surface before being released into the environment [1]. The urea injection system is an essential component of the catalyst NO_x reduction system, with its primary purpose being to atomize the urea solution into fine droplets and ensure uniform distribution throughout the exhaust gas stream. However, when spraying the urea solution into the exhaust pipe, the phenomenon of incomplete evaporation of the urea solution or the contact of the urea stream with the exhaust pipe wall may occur [2]. During urea hydrolysis, while NH_3 is the desired product for the SCR catalyst, undesirable solid by-products, such as biuret, cyanuric acid can also be formed within the liquid film [3], [4]. These solid by-products negatively affect the NO_x reduction performance, hinder the flow of the exhaust gas mixture with NH_3 , and reduce the uniformity of the NH_3 concentration distribution in the gas mixture. The fundamental prerequisite for effective SCR performance is a uniform distribution of NH_3 in the exhaust gas upstream of the SCR unit. Lack of uniformity can cause excess NH_3 , poor NO_x conversion, and catalyst degradation.

Parameters of working modes and installation positions of the injector, such as urea injection pressure, urea injection angle, and urea injection position in the SCR system, have a significant influence on the urea hydrolysis reaction and the uniformity of NH_3 concentration distribution [0], [6]. Suppose the urea injection installation position or spray angle is unreasonable. In that case, urea spraying and hydrolysis will be poor, affecting the NO_x conversion rate, NH_3 distribution uniformity, and urea film or residue on the exhaust pipe wall [7]. In research [8], the authors showed that when the urea injection pressure increased, the average size of urea droplets (Sauter Mean Diameter – SMD) decreased significantly. The decrease in droplet size helped improve the atomization process and increase the evaporation rate of urea, thereby improving the efficiency of NH_3 formation for the selective catalytic reduction reaction (SCR). A CFD study [9] examined urea - SCR spray behavior at low exhaust temperatures. At 180°C , evaporation and pyrolysis are limited, causing stronger wall impingement, uneven NH_3 distribution, and incomplete films. Higher injection pressure and smaller spray angles improve evaporation and droplet uniformity. In study [10], it was found that although injection pressure predominantly governs droplet size, exhaust gas temperature also exerts a significant influence on droplet formation and evaporation. The atomization spray injection induces local cooling, necessitating a higher exhaust gas temperature to achieve complete urea decomposition. Shi et al. [11] reported that proper injection pressure helps prevent wall impingement. At lower pressures, the mixing distance decreases, resulting in a more uniform axial distribution of Urea Water Solution (UWS) droplets. Jeong et al. [12] investigated how injection angle, position, and injector hole number affect ammonia distribution uniformity and conversion efficiency under varying engine loads. The best efficiency occurred with injection perpendicular to the exhaust flow, while 6 - hole and 8 - hole nozzles showed similar performance, both achieving about 95% local evaporation at the monolith face.

Thus, the parameters of the injection process influence the evaporation and hydrolysis of urea solution and the mixing process with the exhaust gas stream, thereby affecting the NO_x reduction efficiency of the NO_x reduction catalyst system. Therefore, the author conducted a study on the influence of urea solution nozzle placement angles (β) on the impact of urea injection with the opposite wall in the exhaust pipe, exhaust gas temperature, and gas mixture uniformity at the SCR catalyst inlet. The simulation is performed on specialized ANSYS Fluent CFD (Computational Fluid Dynamics) software. In which the injection pressure is 0.7 MPa, the urea injector position is kept fixed, and the injection angle (β) compared to the exhaust pipe centerline is changed in 05 cases: $\beta=20^\circ$, $\beta=30^\circ$, $\beta=45^\circ$, $\beta=90^\circ$, $\beta=135^\circ$.

2. METHODOLOGY

2.1. Theoretical basis of simulation in ANSYS Fluent applied to SCR system

This study uses ANSYS Fluent CFD software to simulate the SCR system. The following equations are used:

The mass conservation equation (Continuity equation):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (1)$$

In equation (1): $\mathbf{v}$ represents the velocity of the gas flow (m/s), ρ denotes the density of the gas flow (kg/m³).

The equation of conservation of momentum (momentum equation):

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = - \frac{\partial p}{\partial x} + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} + S_{DPM} \quad (2)$$

In equation (2): p denotes the pressure of the gas flow (Pa), $\rho \mathbf{g}$ is the gravitational force, S_{DPM} represents the source term arising from the interaction with the dispersed phase (in the case of droplets, it corresponds to the reaction force exerted by the droplets on the gas flow) (N/m³), $\boldsymbol{\tau}$ denotes the viscous stress tensor of the gas flow (Pa), determined in equation (3):

$$\boldsymbol{\tau} = \mu_{\text{eff}} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \mu_{\text{eff}} (\nabla \cdot \mathbf{v}) \delta_{ij} \quad (3)$$

In equation (3): μ_{eff} is effective viscosity (Pa.s), δ_{ij} is the coefficient acting on the “main cross” components (xx, yy, zz), when $i = j$ then $\delta_{ij} = 1$ and when $i \neq j$ then $\delta_{ij} = 0$.

The energy conservation equation (energy equation):

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\rho E \mathbf{v}) = -p \nabla \cdot \mathbf{v} + \nabla \cdot (k_{\text{eff}} \nabla T) + S_h \quad (4)$$

In equation (4): ρ denotes the density of the gas flow (kg/m³), E is specific energy of gas flow (J/kg) can be calculated by the formula: $E = h + \frac{v^2}{2}$, h is enthalpy of gas flow (J/kg), $\mathbf{v}$ is the velocity of the gas flow (m/s), p is the pressure of the gas flow (Pa), T is the temperature of the gas flow (K), k_{eff} is effective thermal conductivity (W/mK), S_h is additional energy source

(W/m³). To describe the turbulent characteristics of the gas flow, the RNG k-ε (Re-Normalization Group k-ε) model is applied [13].

The convection - diffusion equation of the i^{th} gas can be expressed as [14]:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (5)$$

In equation

(5): Y_i denotes the mass fraction of the i^{th} gas species in the gas mixture, for example ammonia (NH₃) or other gases involved in the mixing process, ρ is the density of the gas flow, $\vec{v}$ is the velocity vector of the gas flow, $\vec{J}_i$ denotes the diffusion flux vector of the gas species and S_i represents the rate of gas generation due to mass transfer from the dispersed phase and other defined source terms. When these parameters are combined, they describe the overall transport process – including convection and diffusion – of the gases within the computational domain. As a result, the distribution and uniformity of ammonia in the SCR catalyst can be accurately predicted. R_i represents denotes the overall generation rate of gas species i resulting from all chemical reactions. This rate is obtained by summing the products of the molecular weight M_i of species i and the molar rate of its formation or consumption $\hat{R}_{i,r}$ which is determined based on the Arrhenius expression for each reaction r , as expressed by:

$$R_i = M_i \sum_{r=1}^{N_R} \hat{R}_{i,r} \quad (6)$$

In this work, only irreversible reactions were taken into account. Accordingly, the molar rate of formation or depletion of a gaseous species in a specific reaction can be expressed as [14]:

$$\hat{R}_{i,r} = (v''_{i,r} - v'_{i,r}) \left(k_{f,r} \prod_{j=1}^N [C_{j,r}]^{(\eta'_{j,r} + \eta''_{j,r})} \right) \quad (7)$$

As expressed in equation

(7), N indicates the total chemical species within the system, while $v'_{i,r}$, $v''_{i,r}$ correspond to the stoichiometric coefficients related to reactants and products in reaction r . The term $k_{f,r}$ denotes the rate constant of the forward reaction, and $C_{j,r}$ [kmol/m³] gives the molar concentration of species j involved. The parameters $\eta'_{j,r}$ and $\eta''_{j,r}$ refer to the reaction order exponents for the reactant and product sides, respectively. The forward rate constant is determined based on the Arrhenius expression [14]:

$$k_{f,r} = A_r e^{\left(-\frac{E_r}{RT}\right)} \quad (8)$$

In equation (8), A_r refers to the pre-exponential factor and T [K] denotes the absolute temperature. The term E_r [J/kmol] represents the reaction's activation energy, with R being the gas constant having a value of 8314.34 [J/(kmol.K)].

The droplets of the urea solution were tracked in a Lagrangian reference frame using the Discrete Phase Model (DPM) implemented in ANSYS Fluent. After evaporation, the urea decomposes and hydrolyzes:

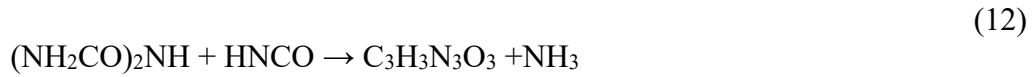


These reactions provide a source of NH_3 for the SCR reaction [15].

Biuret is a common byproduct of urea decomposition, especially when urea is incompletely decomposed under high temperatures:



Generation of cyanuric acid:



The uniformity index (UI) is used to quantify the ammonia (NH_3) concentration distribution at the inlet of the SCR catalyst. The UI value close to 1 indicates that NH_3 is uniformly dispersed over the cross-sectional area at the catalyst entrance. This parameter is derived from a correlation that relates the local and mean NH_3 concentrations near the catalyst surface [16]:

$$\text{UI} = 1 - \frac{1}{2n} \sum_{i=1}^n \frac{\sqrt{(C_i - \bar{C})^2}}{\bar{C}} \quad (13)$$

In equation

(13) n represents the total number of computational cells across the evaluated cross-section, C_i indicates the NH_3 concentration (mass fraction) at the i^{th} cell, while $\bar{C}$ denotes the mean NH_3 concentration (mass fraction) obtained over the entire cross-sectional area. In ANSYS Fluent, the NH_3 concentration at each cell and the average NH_3 concentration over the entire cross-section are output, where NH_3 concentration is expressed as a mass fraction. To export the NH_3 concentration for each cell using the Field Functions tool in Fluent. First, open ANSYS Fluent and load the project that has been created. Then, go to the Reports menu and select Surface Integrals to export the results for each cell. Choose Mass Species Fraction, and select NH_3 . This data can be exported as a table or a CSV file. To calculate the average NH_3 concentration ($\bar{C}$) over the entire cross-section (area-weighted integral method) using the Surface Integrals tool and calculate the total mass of NH_3 over the cross-section, then divide by the cross-sectional area to get the average value. The formula for calculating the average is $\bar{C} = \frac{\int_A c_i dA}{\int_A dA}$, where A is the cross-sectional area. Finally, after calculating and displaying the NH_3 concentration at the cells and averaging it over the cross-section, the results can be saved as a .csv or .txt file for further analysis or calculations.

2.2. Simulation model and input parameters

The exhaust pipe section containing the urea injector and the SCR catalyst with the structure shown in Figure 1 is simulated.

These parameters taken from the experiments on a D4BB diesel engine at 50% load, 75% load, 100% load at speed of 2000 rpm are shown in Table 2.

Tab. 2

Parameters measured

Parameters	Value at 50% load	Value at 75% load	Value at 100% load	Unit
Exhaust gas inlet temperature	511	627	735	K
Urea solution temperature	300	300	300	K
Exhaust gas velocity inlet	6.77	6.83	7.03	m/s
Urea injection velocity	32.54	32.54	32.54	m/s
Pressure at exhaust inlet	0.12	0.125	0.13	MPa
Urea injection pressure	0.7	0.7	0.7	MPa
Pressure at the exhaust outlet	0.1	0.1	0.1	MPa
Urea solution density [19]	1090	1090	1090	kg/m ³
Exhaust gas density [20]	1.2943	1.2943	1.2943	kg/m ³
Thermal conductivity (Urea solution)	0.0242	0.0242	0.0242	W/m.K
Thermal conductivity (Exhaust gas)	0.0626	0.0626	0.0626	W/m.K
Urea injection angle	20	20	20	Degree
Urea injection angle	30	30	30	Degree
Urea injection angle	45	45	45	Degree
Urea injection angle	90	90	90	Degree
Urea injection angle	135	135	135	Degree

2.3. Model meshing

The 3D model and meshing model are shown in Figure 3. In this study, the mesh was generated using an unstructured hybrid mesh with structured quadrilateral and triangular mesh elements – a popular choice in heat transfer problems, turbulence, and complex flow simulations, which helps to improve computational accuracy and increase the convergence speed of the solution.

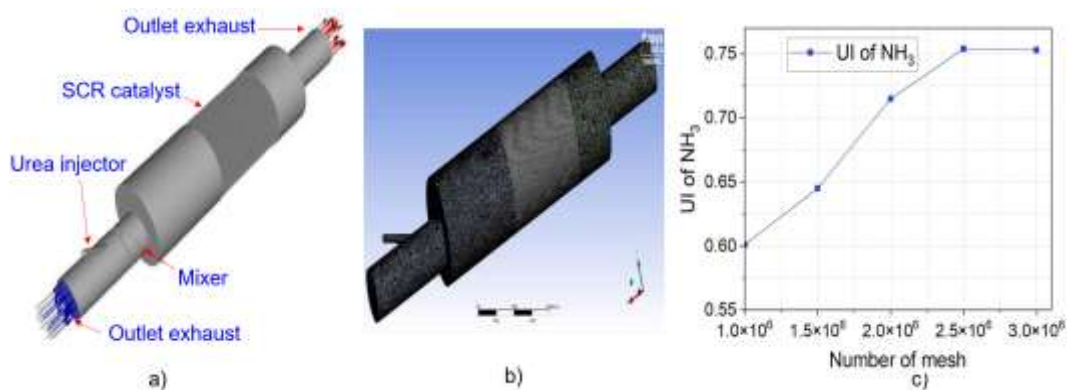


Fig. 3. 3D model meshing a) 3D model, b) 3D model meshing, c) Comparison of UI of NH_3 with a different number of meshes

The mesh element size of the model surface is set in the range of 2-8 mm at different positions throughout the entire exhaust pipe section. To evaluate the impact of grid resolution on the ammonia uniformity index, four computational meshes containing 1.0, 1.5, 2.0, 2.5, and 3.0 million elements were tested. The problem was simulated for 600 steps. The results showed that when using a mesh of 2.5 million elements, the UI of NH_3 did not change significantly and reached the highest value of 0.754 (Figure 3c).

The skewness metric was evaluated for three element types: Tet4, Hex8, and Wed6. As shown in Figure 4, most elements have low skewness values. The majority of Hex8 elements exhibit skewness below 0.1, while Tet4 elements are mainly concentrated in the range of 0.1-0.3. The fraction of elements with skewness greater than 0.5 is tiny, and no aspect exceeds 0.8. These values lie well within the recommended limits in ANSYS Fluent (skewness < 0.85), indicating a low level of element distortion and thereby supporting good accuracy of the CFD solution.

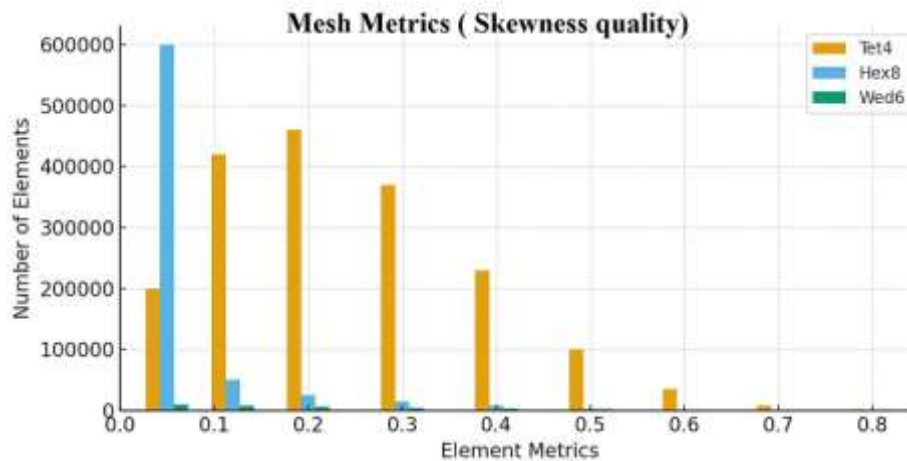


Fig. 4. Skewness quality distribution for 2.5 million mesh elements

To assess the orthogonality of the mesh, the orthogonal quality metric was also calculated. As illustrated in Figure 5, its values range from about 0.2 to nearly 1, with an average of approximately 0.84. In particular, most Hex8 elements have orthogonal quality values close to 1, demonstrating perfect orthogonality of the mesh. Only a small number of Tet4 elements exhibit lower orthogonal quality, but they remain within the acceptable range. With all elements above the minimum threshold of 0.15, the mesh exhibits good orthogonality, ensuring reliability and stability for both flow and heat transfer simulations.

Based on this analysis, approximately 2.5 million mesh elements were employed in the simulation domain.

3. RESULTS AND DISCUSSION

3.1. Effect of urea injection angle on urea impingement on the exhaust pipe wall

To evaluate the possibility of urea injection hitting the opposite wall in the exhaust pipe, five exhaust pipe models with urea injection angles of 20°, 30°, 45°, 90°, 135° were simulated (Figure 6). Simulation results show that when the urea injection angles $\beta = 20^\circ, 30^\circ$ the injection jet is directed nearly parallel to the movement of the exhaust flow, helping the urea and NH_3

particles to disperse along the length of the pipe, limiting the phenomenon of impact on the pipe wall, and creating conditions for more even mixing with the exhaust flow. In addition, arranging the injection jet to move in the same direction as the exhaust flow will help reduce fluid loss and improve the mixing process between the spray solution and the exhaust flow throughout the pipeline. When the urea injection angles $\beta = 45^\circ$, 90° and 135° the injection solution will directly collide with the opposite wall of the exhaust pipe. This will cause the solid by-products, such as biuret, cyanuric acid, to form from the liquid film and deposit on the pipe wall. The deposited urea is difficult to evaporate and mix with the exhaust flow. Therefore, it reduces the amount of urea participating in the hydrolysis reaction, thereby reducing the efficiency of NO_x reduction in the exhaust flow.

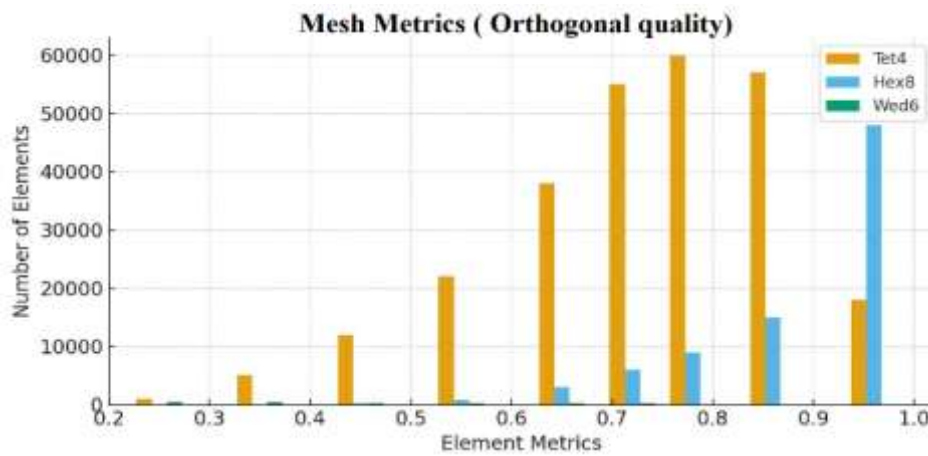


Fig. 5. Orthogonal quality distribution for 2.5 million mesh elements

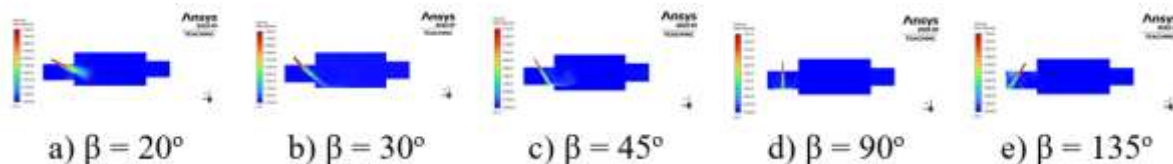


Fig. 6. Influence of urea injection angle on wall impingement in the exhaust pipe

3.2. Influence of urea injection angle on the temperature of the gas mixture at the SCR catalyst inlet

Figure 7 illustrates the temperature distribution of the exhaust gas and urea combination at the intake of the SCR catalyst. It was observed that the exhaust temperature at the inlet of the SCR catalyst rises progressively as the engine load increases. For example, at 2000rpm with $\beta = 30^\circ$, the temperature is about 452.13K at 50% load, rises to 568.11K at 75% load, and reaches 676.23K at 100% load.

Gas mixture temperature at the SCR catalyst inlet in all cases is in the range of 444.28K÷677.21K, which is within the effective working range of the SCR catalyst [21]. Figure 7 also shows that with the injection angle $\beta = 20^\circ$, the temperature of the gas mixture at the SCR catalyst inlet reaches the highest value 677.21K at 2000 rpm, 100% load mode. When the injection angle $\beta = 20^\circ$ produces a spray that is more aligned with the main exhaust flow, resulting in weaker spray – wall impingement and reduced lateral penetration. Consequently,

the droplets experience a shorter residence time near the wall and a smaller liquid – gas contact area. These factors lead to less evaporative cooling, allowing the hot core flow to be better preserved at the SCR inlet. Sufficiently high and evenly distributed temperature at the SCR catalyst inlet will promote the pyrolysis and hydrolysis of urea, helping to generate more NH_3 evenly, thereby improving the NO_x reduction efficiency. As the injection angle is increased, the radial velocity component of droplets increases, enhancing the probability of collision and rebound with the pipe wall [22]. These zones trap evaporatively cooled gas and mix it back into the main stream, resulting in greater cooling and a lower area-averaged temperature at the SCR inlet.

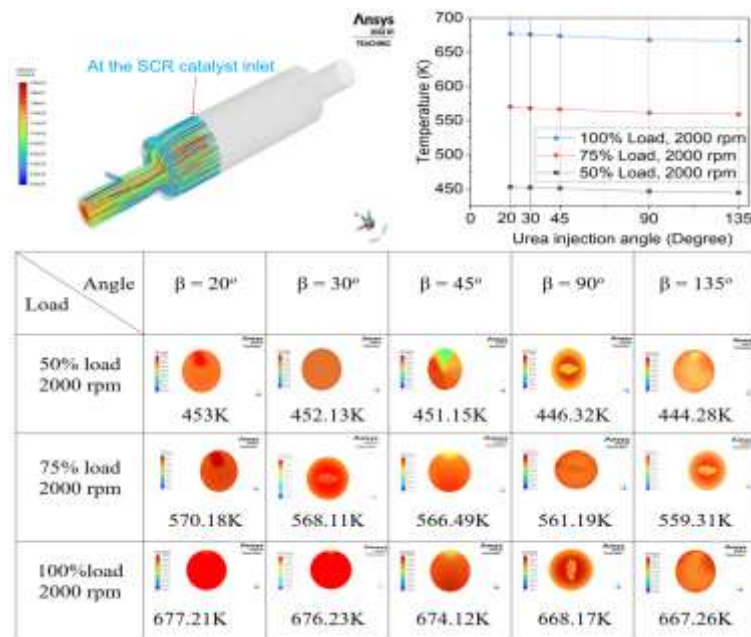


Fig. 7. Temperature of the gas mixture at the SCR inlet for various urea injection angles

3.3. Effect of urea injection angle on the uniformity of NH_3 /gas mixture at the SCR catalyst inlet

In the SCR system, the NO_x conversion efficiency is strongly influenced by the uniformity of the NH_3 in the gas mixture before entering the catalyst. When NH_3 is evenly distributed, the entire catalyst surface receives the necessary amount of reductant; thereby the reaction with NO_x takes place effectively, the reduction efficiency reaches near the maximum value, and the phenomenon of NH_3 slip is limited. On the contrary, if NH_3 is unevenly distributed, areas lacking NH_3 will not completely reduce NO_x , while regions with excess NH_3 will increase the risk of NH_3 slippage, causing secondary emissions. Therefore, the more uniform the NH_3 distribution in the gas mixture is, the higher and more stable the NO_x conversion efficiency of the SCR system will be.

Figure 8 illustrates the variation in the NH_3 uniformity index (UI) with respect to urea injection angle across three load conditions of 50%, 75%, and 100% at 2000 rpm. As the engine load increases, the NH_3 uniformity index (UI) shows a clear upward trend, reaching its maximum at full load (100%), followed by 75% and 50%. This is explained by the fact that when the load increases, the temperature and exhaust gas flow increase, helping the evaporation and mixing of NH_3 in the gas stream to take place more strongly, increasing the uniformity of

the mixture. Regarding spray angle, UI increases rapidly from 20° to 30° and reaches a maximum value at a urea injection angle of 30° , then gradually decreases as the spray angle continues to increase. The reason is that when the spray angle is too slight, the spray is concentrated and the coverage area is narrow; while when the angle is too large, the spray collides with the pipe wall earlier, reducing the mixing efficiency. Thus, the urea injection angle $\beta = 30^\circ$ is considered optimal to achieve the highest uniformity of NH_3 at the investigated urea injection angles β and the investigated loading mode. In addition, in the study of S. Jeong et al. [17], with the distance from the injector to the front cross-section of the SCR being 400 mm and the exhaust gas velocity from 6 to 12 m/s, corresponding to the residence time ranging from 0.03 s to 0.06 s, with a UI value of 0.733. In our study, this distance was shortened to 350 mm, with an exhaust gas velocity from 6 to 7 m/s, resulting in a residence time of about 0.05 s and a maximum UI value of 0.826, showing a significant improvement in the efficiency of mixing and dispersing the exhaust gas flow while improving the accuracy of the simulation model.

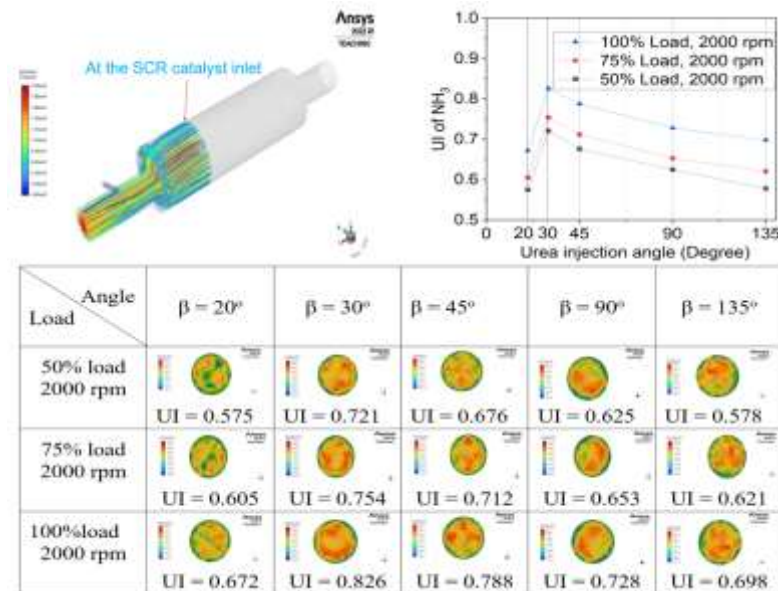


Fig. 8. Uniformity Index of NH_3 at the SCR Catalyst inlet for different urea injection angles

4. CONCLUSIONS

In this study, an SCR design model was developed in which the length from the urea injector to the SCR catalyst inlet was chosen to be 350 mm based on the recommendation that 200-400 mm would be sufficient for complete hydrolysis of the urea solution in NH_3 at a similar exhaust gas flow rate, as published in [17]. Based on this model, a SCR 3D model was constructed in ANSYS Fluent using a 2.5 million-element mesh to ensure a stable UI value. The first novelty of this research was that exhaust gas temperatures, pressures, density, velocities, and flow rates; urea solution temperature and density; urea injection velocity, pressure, and urea injection angles for the D4BB engine were measured on an engine test bench under load characteristics at 2000 rpm to provide input data for the ANSYS Fluent simulation model.

The second novelty is that when the urea injection angle β is 20° and 30° , the amount of sprayed solution colliding and sticking to the exhaust pipe wall is reduced, thereby reducing the amount of urea sticking and decomposing on the pipe wall surface; simulations and comparisons were carried out for five different angles, including 20° , 30° , 45° , 90° , 135° .

The third novelty is the provision of a data set on the temperature distribution of the exhaust gas and urea mixture at the inlet of the SCR catalyst, which varies depending on the engine's operating characteristics. In this case, the temperature of the gas mixture at the inlet of the SCR catalyst is in all cases within the range of 444.28 K - 677.21 K, which corresponds to the effective operating range of the SCR catalyst recommended in [21].

Experimentally determining the homogeneity of NH_3 in the gas mixture before entering the catalyst requires expensive measurement equipment, complex experiments, and is often impossible. Therefore, the use of modeling tools such as CFD is an effective solution, which has been implemented in published work by other authors [10], [12], [17] and [22] as well as in this study. The final novelty is that at an ure injection angle $\beta = 30^\circ$, the NH_3 distribution at the SCR catalyst inlet is more uniform compared to the other injection angles, thereby enhancing the homogeneity of NH_3 and exhaust gas mixture upon entering the catalyst and improving the catalyst's NO_x conversion efficiency.

In future studies, the obtained results will serve as a basis for designing and manufacturing an exhaust pipe section for installing a urea solution injector, specifically, and an SCR system, generally, for in-use diesel engines without SCR systems.

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