

Dosing Control of Urea in Selective Catalytic Reduction (SCR) to Enhance the Reduction of Nitrogen Oxides

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Abstract

Selective Catalytic Reduction (SCR) is an effective aftertreatment technique designed to comply with rigorous emission criteria established by global regulatory authorities for the elimination of nitrogen oxides from exhaust streams. Since NO_x and ammonia reagents are poisonous and an excess of either is therefore very undesired, it poses an intriguing control problem, particularly at high conversion. SCR systems must reduce NO_x emissions as much as possible and reduce the possibility of solid deposit fouling, which can harm both the engine and the SCR system. The injection and vaporization of the urea, as well as the diffusion of ammonia in the exhaust gases, have a major impact on both Undecomposed urea can cause solid deposits to form, which unpleasantly impact system performance by raising back pressure of engine and lowering overall fuel efficiency. Two SCR models were evaluated: a base and a revised model, both simulated using CFD. The revised design demonstrated a significant 48.8% reduction in accretion rate and better NO_x reduction performance, while compared with base model. Incorporate the hybrid mixer to enhance the SCR system efficiency in revised SCR model, compares the two optimized designs of Hybrid mixers. Mixer 1 design is better suitable to reduce the solid deposits and enhance the SCR system performance. The mixer 1 design achieves 4% reduction in accretion rate compared with mixer2 design of hybrid mixer in revised SCR model.

Keywords: Solid Deposits, Selective Catalytic Reduction, Mixer design, After treatment system, mixer design, NO_x reduction, optimized design

INTRODUCTION

Selective Catalytic Reduction

Selective Catalytic Reduction (SCR) systems are highly effective in reducing NO_x emissions from vehicle exhaust, particularly in diesel engines. This advanced technology involves injecting a reducing agent, such as urea or ammonia, into the exhaust stream. The chemical process converts the harmful NO_x gases into nitrogen and also water vapor, which are harmless to the environment. SCR systems are recognized for their ability to achieve high NO_x reduction efficiencies, often exceeding 90%, making them a vital component in meeting stringent emission regulations [1, 2]. Furthermore, SCR technology helps to improve fuel combustion efficiency and reduce greenhouse gas emissions.

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According to the International Energy Agency (IEA), the automobile sector contributes significantly to air pollution, making up to 24% of worldwide CO₂ emissions from fuel combustion [3, 4]. These emissions consist of a range of pollutants, including carbon dioxide, sulfur oxides, nitrogen oxides and particulate matter. Nitrogen oxides (NO_x) are formed primarily through high-temperature combustion processes in internal combustion engines and include nitrogen monoxide (NO) and nitrogen dioxide (NO₂) [5]. Their formation occurs when nitrogen and oxygen in the

air react under high-temperature conditions during combustion. Nitrogen oxides (NO_x) interact with the environment and also humans in ways that pose significant challenges [6]. Their actions cause ground-level ozone and particulate matter to form, which are both bad for people's health and the environment.

(SCR Technology)

Selective Catalytic Reduction (SCR) systems are used in diesel engines to reduce nitrogen oxides (NO_x) emissions by employing ammonia as a reduction agent. The composition of an SCR system typically includes catalysts such as vanadium oxide (V₂O₅) or iron zeolites, which are supported on a ceramic substrate to facilitate the reduction reaction and improve efficiency [3, 7]. SCR systems are critical in meeting stringent emission standards, significantly reducing the harmful pollutants in exhaust gases [8]. The use of urea or ammonia ensures effective NO_x reduction, enhancing engine performance and contributing to environmental sustainability.

Working of SCR System

SCR systems are typically composed of the following main components: Diesel Oxidation Catalyst (DOC), which oxidizes carbon monoxide, hydrocarbons into carbon dioxide plus water, while also converting some of the nitrogen oxides (NO) into nitrogen dioxide (NO₂); an AdBlue (Urea Solution) Tank that stores the aqueous urea solution, typically 32.5% urea in water [9, 10]. Fig 1 represents the detailed view of the engine aftertreatment system with SCR, DOC, and DPF. The diesel particulate filter helps to reduce the soot and particular matters. An AdBlue Dosing System that precisely meters and injects the urea solution into the exhaust gas using a specialized nozzle or injector; the SCR Catalyst, which is the heart of the system and facilitates the reaction between the injected ammonia and nitrogen oxides, converting them into harmless nitrogen and water vapor [11]. Sensor and Control Module, which includes various sensors and an electronic control module that monitor the system's operation and adjusts the urea injection rate based on factors like engine load, speed, and exhaust temperature [4, 12].

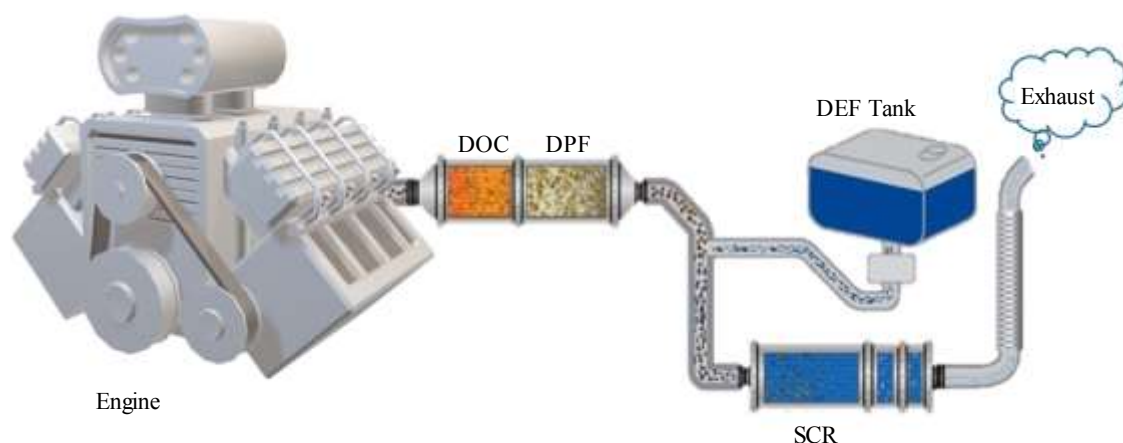


Figure 1. Engine with aftertreatment SCR system.

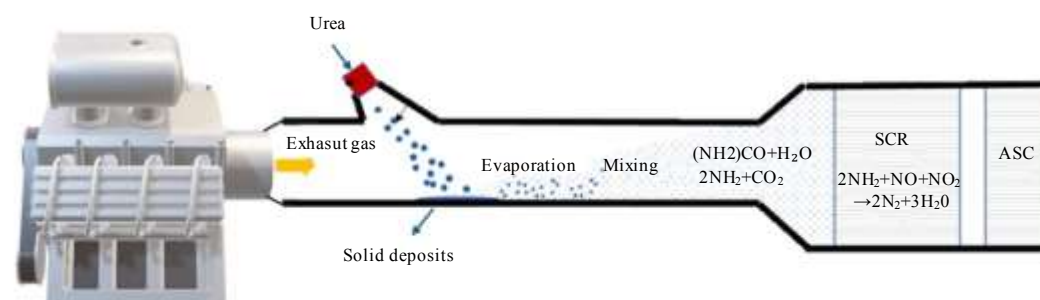


Figure 2. Solid deposits formation in SCR system.

Solid Deposit Formation

The incomplete urea decomposition or improper injecting urea in exhaust gases causes solid deposits formation within the SCR system, as shown in Figure 2 [13, 14]. These deposits can accumulate on the catalyst surface, mixer components, or exhaust piping, potentially clogging the system and reducing its efficiency [15]. Deposit formation can result from factors such as inadequate temperature conditions, insufficient residence time for urea breakdown [16]. Regular maintenance and proper operating conditions are necessary to mitigate deposit formation and preserve the performance of the SCR system.

INTRODUCTION TO THE MIXERS IN SCR SYSTEM

Selective Catalytic Reduction is at the forefront of emission reduction technologies, particularly for diesel engines. These systems work by introducing a urea solution into the exhaust gases, which decompose into ammonia, thereby significantly reducing harmful emissions. However, for the process to be effective, the ammonia must be uniformly distributed within the exhaust stream, which is where mixers play a crucial role. The primary function of the mixer is to enhance the homogeneity of the injected urea or ammonia with the exhaust gases. Effective mixing ensures that the reactants are uniformly dispersed across the exhaust flow, facilitating consistent and efficient catalytic reactions [5]. Without a mixer, the uneven distribution of urea could lead to localized over- or under-dosing of ammonia, resulting in poor NO_x conversion rates and potential ammonia slip (unreacted ammonia passing through the system).

Beyond mere distribution, mixers also serve to break up larger droplets of injected urea, assisting in the evaporation and decomposition processes [17]. This makes mixer design critical for achieving optimal SCR performance, reducing the risk of undesired side reactions or incomplete decomposition that could lead to deposit formation or inefficiency in NO_x reduction.

Importance of Mixer in SCR Performance

Mixer geometry is vital because it directly influences the entire efficiency of the SCR system. The structure of the mixer, including the shape and arrangement of blades or mixers, determines how well it can induce turbulence in the exhaust flow [5]. Higher turbulence levels promote better mixing and more effective interaction between the ammonia and NO_x, leading to a higher conversion efficiency in the catalyst [6]. In addition to geometry, the placement of the mixer within the SCR system is crucial. It must be located at a point where sufficient mixing can occur before the flow reaches the catalyst. The interaction between the mixer and the exhaust flow path, including factors like residence time and flow velocity, are essential considerations. Poor placement can result in uneven ammonia distribution, leading to hot or cold spots in the catalyst, which reduces the overall effectiveness of the system [18]. Furthermore, the mixer's impact on pressure drops across the SCR system cannot be overlooked. A well-designed mixer should provide the necessary mixing without causing excessive pressure losses, which could affect engine performance and fuel efficiency [19]. Therefore, mixer design must strike a balance between enhancing mixing and minimizing pressure drops, making it a critical factor in optimizing SCR performance.

Reductants

Air pollutants known as nitrogen oxides (NO_x) are extremely reactive and can have a negative impact on the environment and human health. The reductants or reducing agents plays a crucial role in the developments in SCR technology and their NO_x reduction. The various reductants used in SCR systems are hydrogen, carbon monoxide, hydrocarbons, and ammonia/urea [20]. The ability of ammonia, which is well known for its effectiveness in SCR, to lower NO_x emissions was investigated. A low-toxicity and safe substitute is urea-based SCR, especially for mobile applications. Because of their versatility, hydrocarbon-based SCR systems can operate at lower temperatures and with greater efficiency. An environmentally favorable solution for reducing NO_x is hydrogen-based SCR technology, especially in low-temperature situations [21].

Injection pattern of reductants improves the uniformity of the concentration distribution in the

exhaust flow [22].

SYSTEM GEOMETRY AND METHODOLOGY

Creation of SCR Design

The base design typically includes the exhaust inlet, catalyst bed, and exhaust outlet. The geometry should capture essential features such as the flow path and catalyst arrangement. Creating the geometry for an SCR system is a critical step in the CFD simulation process. Once the geometry is created, it needs to be imported into meshing software. Common meshing tools include ANSYS Meshing, ICEM CFD, and Gambit. To preserve the design's integrity and prevent any details from being lost that could compromise the simulation's correctness, the geometry must be imported accurately [23]. The geometry details for the SCR system must include both the base and revised designs [24]. The base design generally consists of the basic components without any additional modifications, while the revised design may include enhancements such as hybrid mixers.

The revised design includes modifications such as optimized catalyst shapes, the addition of mixers, and improved injector placements to enhance performance.

Hybrid mixers are critical as they help in the thorough mixing of the exhaust gases with the injected urea, leading to improved reduction of NO_x emissions. Ensuring that the hybrid mixers are accurately represented in the geometry is vital for the simulation to capture their impact on the flow and chemical reactions. Figure 3 and 5 illustrates the base design and revised design with dimensions [24].

The urea injector is located 407 mm upstream from the catalyst inlet with 45° injection angle as shown in Figure 4 for base SCR model.

In revised model, the urea injector is located parallel to exhaust flow for better atomization as shown in Figure 6 for base SCR model.

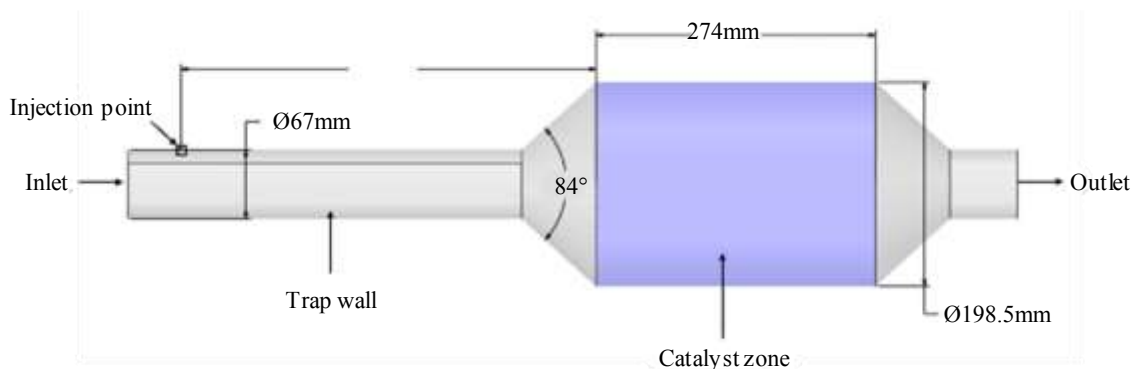


Figure 3. Base design configurations.

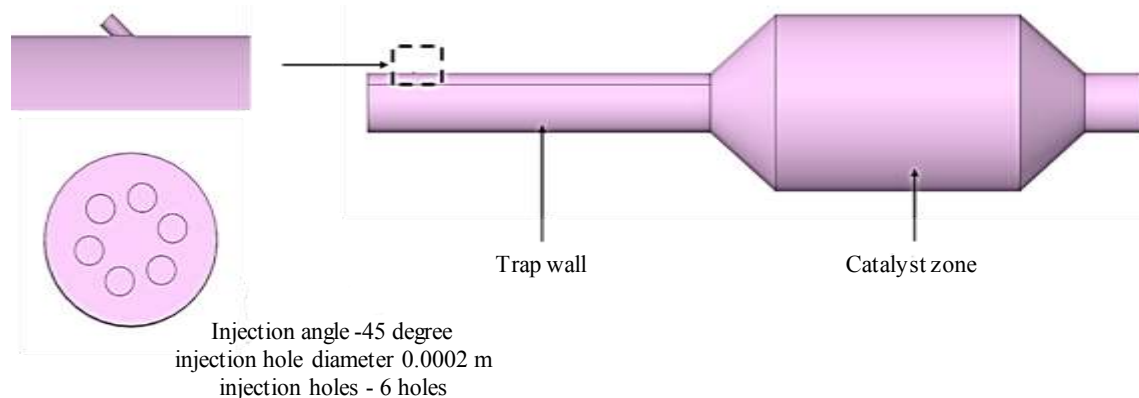


Figure 4. Urea injector in base model.

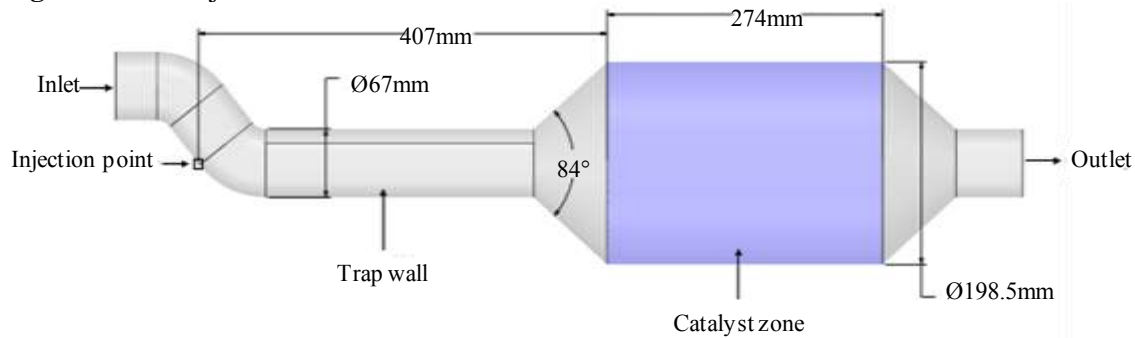


Figure 5. Revised design configurations.

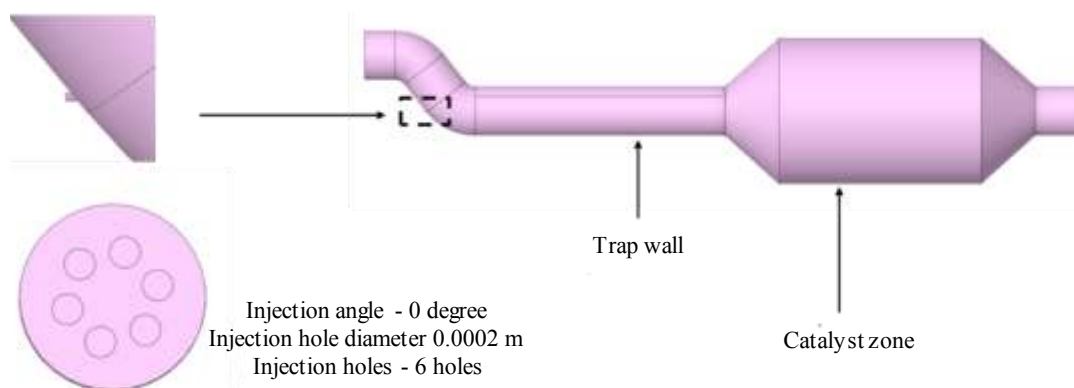


Figure 6. Urea injector in revised model.

The revised design incorporates hybrid mixers placed upstream of the catalyst. These mixers are strategically added to improve the dispersion of injected urea and enhance the mixing of exhaust gases. By promoting better interaction between the urea and the exhaust flow, the mixers help ensure a more uniform distribution of the reducing agent, leading to more efficient reactions within the catalyst. By improving the conversion of nitrogen oxides (NO_x) and reducing the production of undesirable byproducts, this mixing innovation raises the SCR system's overall efficiency.

Integration of Hybrid Mixer

The hybrid mixer design integrates both features of swirl and flap mixers into a specific unit, positioned in one diameter of inlet pipe downstream from the injection point of urea. This model aims to maximize the mixing efficiency of ammonia and exhaust gases while minimizing urea deposition and enhancing overall flow uniformity [24]. By combining the best features of both mixer types in one configuration, the hybrid mixer offers a high-performance solution for improving SCR system efficiency while keeping pressure drop within acceptable limits. So, the hybrid blade is created into two different mixer designs for evaluation. Mixer 1 design includes the outer ring layer for swirl blades as shown in Figure 7. Mixer 2 design includes flap blades in middle and incorporates the swirl blades around it as shown in Figure 8.

Properties and Fluid Specifications

Specifying the material properties and fluid specifications is essential for accurate CFD simulations. The materials involved in the SCR system, such as the catalyst, should have their properties defined, including density, thermal conductivity, specific heat, and porosity. These properties affect heat transfer and chemical reaction rates. The fluid properties include the properties of the exhaust gases, urea, and ammonia. Its properties such as density, viscosity, and specific heat are temperature-dependent and must be specified accordingly. For the urea solution, it is modeled as a multicomponent liquid that breakdown into ammonia and isocyanic acid upon injection. The evaporation and chemical reaction rates of urea need to be specified, considering factors such as temperature, pressure, and the presence

of catalysts.

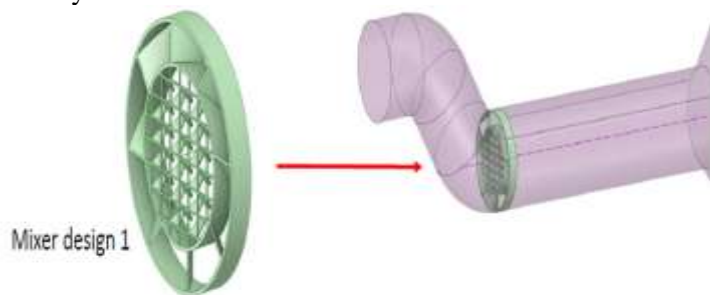


Figure 7. Mixer 1 design insert in revised model.

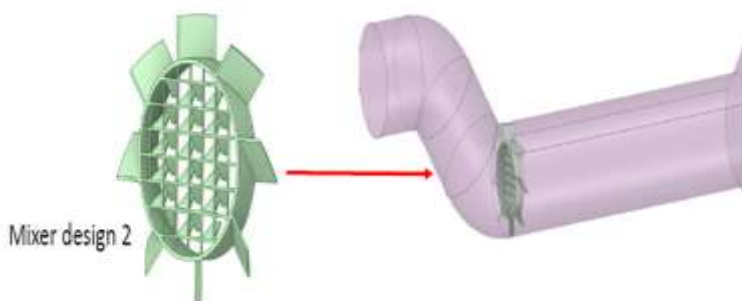


Figure 8. Mixer 2 design insert in revised model.

Injection Condition

The injection process was characterized by a spray velocity of 27 m/s and a spray pressure of 5 MPa, with urea flow rates set at 19.6 mg/s [24]. The injection flow consisted of a multicomponent mixture of urea and water, with mass fractions of 0.325 and 0.675, respectively. These parameters define the initial spray dynamics, ensuring precise modeling of droplet breakup, evaporation, and subsequent chemical reactions. The specified conditions also serve as the baseline for fluid flow and species transport, facilitating accurate simulation and analysis of the SCR process. Additionally, the generation of NH_3 is directly impacted by the interaction of spray velocity and flow rates, which also affects the homogeneity of urea dispersion across the catalyst surface.

RESULTS AND DISCUSSION

The total pressure drop is calculated for each mesh configuration, providing key insight into the flow characteristics and resistance within the system. The results are then compared to assessing the impact of mesh density on the pressure drop predictions, helping to determine how fine the mesh should be for accurate results.

Analysis Between Base and Revised SCR Model

Both the base and revised SCR designs' velocity, pressure distributions were assessed. The performance of the revised design is noticeably better than that of the base design when comparing the two designs. The revised design's S-bend intake and moved injection point improve exhaust gas distribution and lessen catalyst surface deposition. Improved flow homogeneity across the reactor reduces urea accumulation and increases NO_x reduction efficiency. The revised design improves overall system efficiency by addressing the main problems with the base design, namely greater deposition rates and uneven flow. Figure 9 illustrates the Urea injection pattern in Base SCR Design and Figure 10 illustrates the Urea injection pattern in Revised SCR Design.

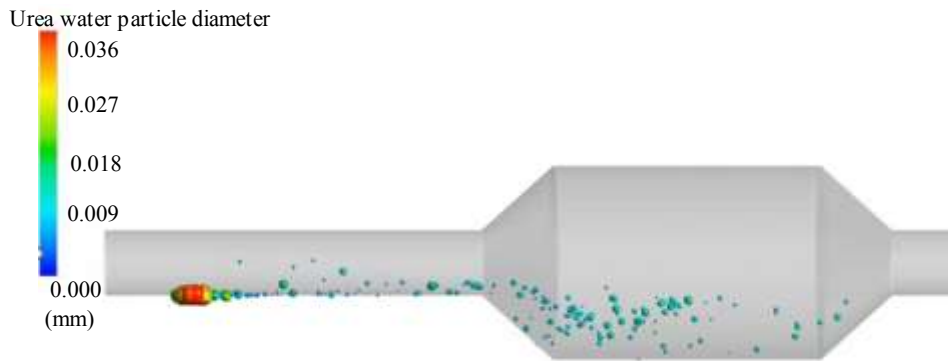


Figure 9. Urea injection pattern in base SCR design.

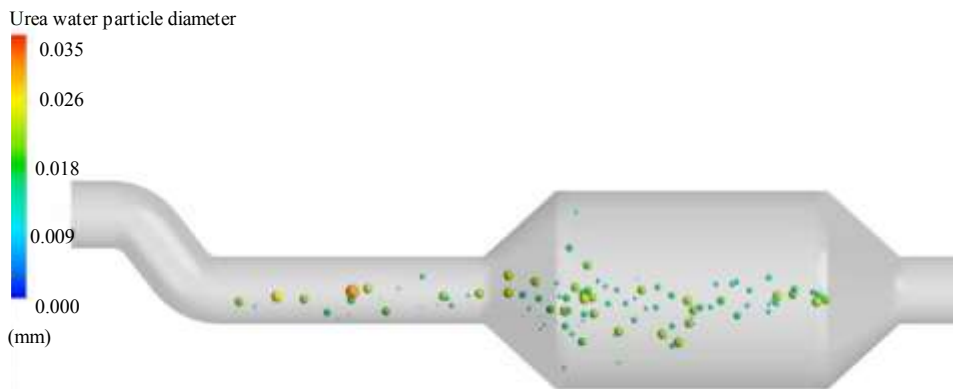


Figure 10. Urea injection pattern in revised SCR design.

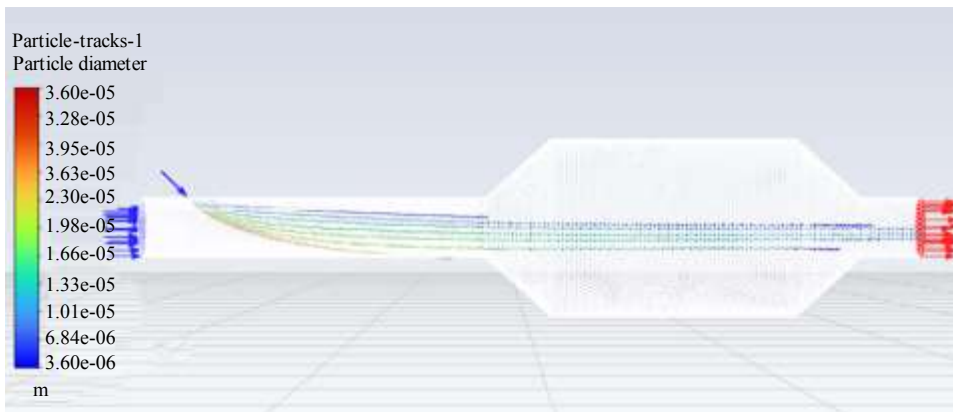


Figure 11. Urea particle path in base SCR Design.

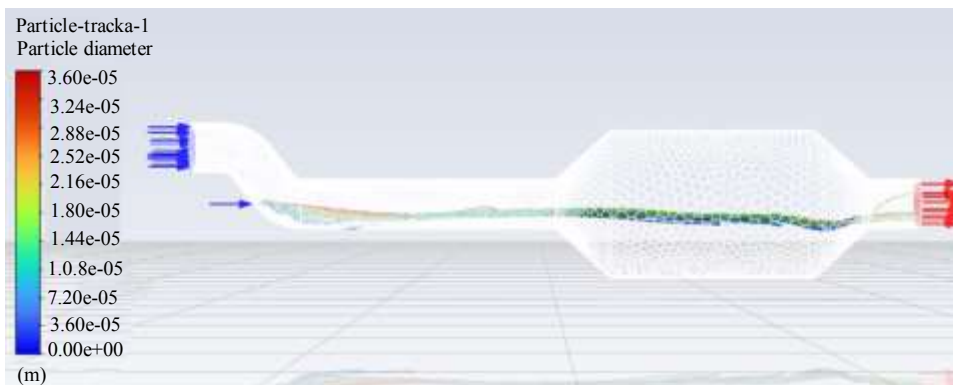


Figure 12. Urea particle path in revised SCR design.

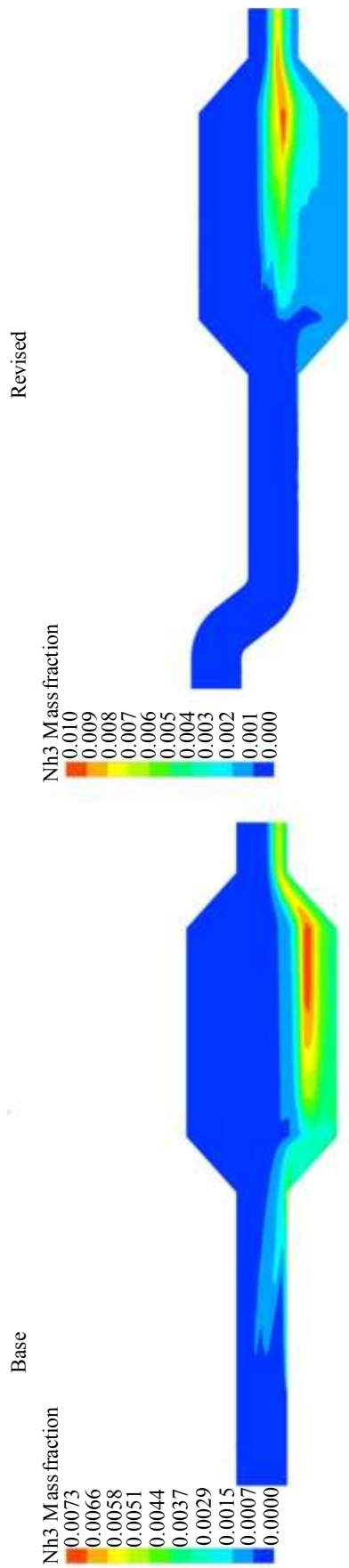


Figure 13. Ammonia mass fraction of base & revised SCR design.

Enhanced ammonia blending and improved NO_x reduction were made possible by the revised design's smoother flow patterns, more effectively pressure distribution, and optimum temperature profiles. Figure 11 illustrates the Urea particle path in Base SCR Design and Figure 12 represents the Urea particle path in Revised SCR Design. In comparison to the base design, the revised design produced a more uniform velocity field, as indicated by the mid-plane NH₃ mass fraction magnitude.

The study of particle interaction looks at how urea particles move and behave as they pass through the system. The research emphasizes how the distribution, melting, and particle size of the urea molecules are influenced by their interactions with the exhaust gas flow. The influence of system adjustments on urea dispersion and deposition is demonstrated by particle pathways between the base and revised models. To improve urea circulation, lessen urea solid deposition, and boost system efficiency overall, this interaction study aids in the optimization of design elements. The revised design reduces deposition on surfaces and strives for consistent particle dispersion. Figure 13 illustrates the Ammonia Mass fraction of Base & Revised SCR Design and Figure 14 represents Ammonia Mass fraction at Inlet & outlet of Base & Revised SCR Design.

Analysis of Mixer 1 And Mixer 2 Designs

The Hybrid mixer which includes advantage of swirl and flap blade design features. So executed the analysis on these two mixer 1 & 2 designs for better optimized mixer design, accretion rate of Mixer 1 design value 1.1×10^{-4} kg/m².s and accretion rate of Mixer 2 design value 2.90×10^{-5} kg/ m².s as shown in Figure 15 [24]. It shows that the hybrid mixer improves mixing.

The urea solid deposit thickness of Mixer 1 design was 2.6×10^{-4} microns and Mixer 2 design was 7.80×10^{-5} microns as shown in Figure 16 [24].

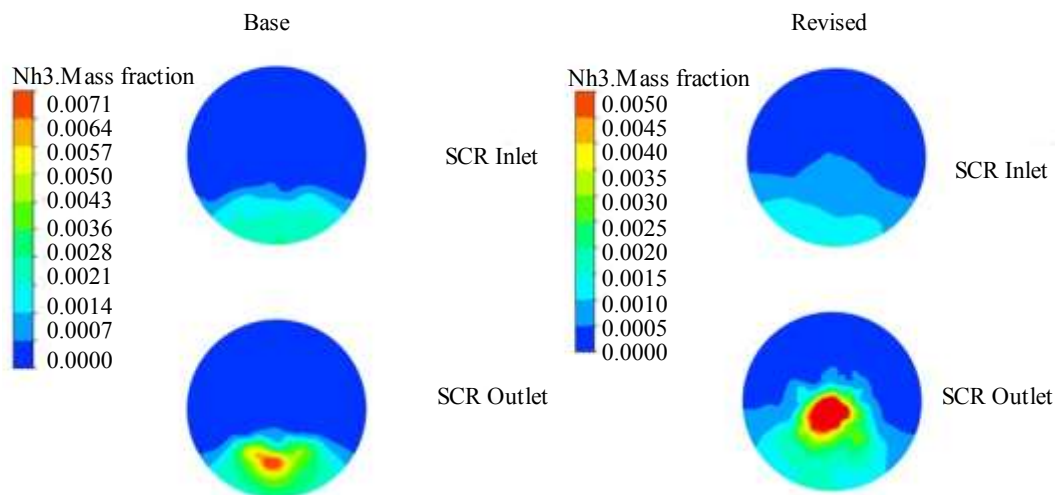


Figure 14. Ammonia mass fraction at inlet & outlet of base & revised SCR design.

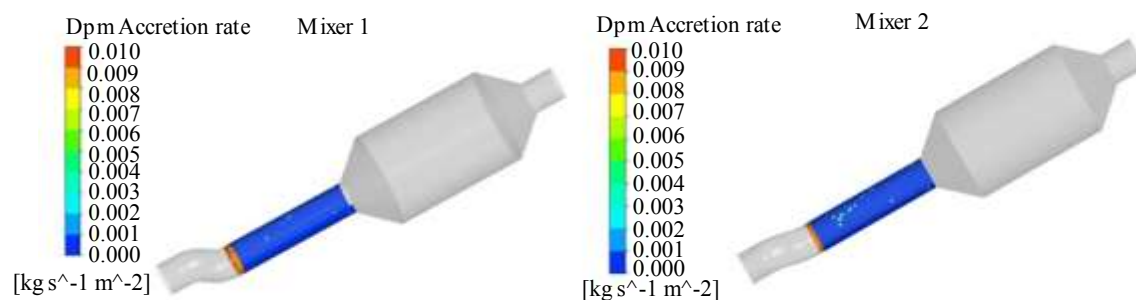


Figure 15. Accretion rate comparison between Mixer 1 and Mixer 2 of Hybrid blade designs.

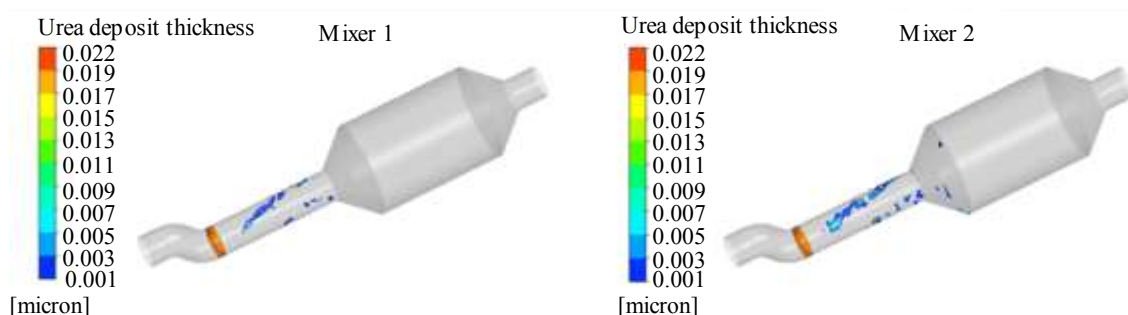


Figure 16. Urea solid deposit thickness comparison between Mixer 1 and Mixer 2 of Hybrid blade designs.

According to the simulation results, the Mixer 1 design is the best design for lowering urea deposit thickness and accretion rates while keeping a high NH_3 mass fraction at the inlet and outlet. When compared to mixer 2 design, simulation findings show that the hybrid mixer, Mixer 1 design, is the most efficient option for lowering accretion rates and urea solid deposit thickness.

CONCLUSION

This study examined how well design changes and mixing technologies improved the performance of SCR systems. The revised design with an S-bend intake and a repositioned injection point greatly decreased urea deposition and enhanced flow distribution, while the base design showed excessive accretion rates and inadequate NO_x conversion. The accretion rate was lowered by 48.8% due to the S-bend inlet and relocated urea injection in revised SCR design. The best option for improving SCR performance turns out to be the hybrid mixer. When compared to mixer 2 design, mixer 1 design is the most efficient arrangement for lowering accretion rates and urea solid deposit thickness, its reduces 4% accretion rate.

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