3D NUMERICAL ANALYSIS FOR OPTIMIZATION OF UREA-SCR PERFORMANCE IN MARINE DIESEL ENGINE

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ABSTRACT

Due to the increased awareness of negative impacts of nitrogen oxides on health and environment, IMO has issued stringent regulations to control NO\textsubscript{x} in diesel exhaust emitted from operating marine vessels. In order to comply with these regulations, a large amount of research was performed to develop NO\textsubscript{x} after-treatment technologies and SCR is one of the most proven mainstream techniques to reduce NO\textsubscript{x} emission in heavy duty diesel engines.

This paper presents a numerical optimization approach for SCR system performance in order to achieve higher NO\textsubscript{x} reduction efficiency in marine diesel engine. The performance of SCR system is analyzed using ANSYS Fluent 15. The geometry is created in ANSYS workbench and mesh is generated in ANSA. Two parameters are examined for evaluating SCR performance namely urea conversion efficiency, and Stoichiometric Area Index (SAI) in terms of two injection specifications which are not possible to experimentally detect namely droplet size (SMD), and injection velocity at different exhaust gas velocities. In this work, we proposed a new evaluation parameter SAI, for projecting the active range area of NH\textsubscript{3}/NO molar ratio (0.8-1.2) that helps in understanding the process development. Based on this, a blade static mixer is installed upstream of SCR entrance at different exhaust gas velocities in order to promote urea to ammonia conversion for further improvement in NO\textsubscript{x} conversion efficiency.

It is observed that relatively small-sized droplets are required to achieve the maximum urea conversion efficiency and SAI due to better UWS droplet atomization and enhanced evaporation. Evaluation parameters are also enhanced at elevated injection velocities due to better mixing with exhaust flow. However, higher injection velocity will have negative effect on spray distribution due to small residence time leading to less chemical interaction between ammonia and oxides of nitrogen in exhaust gas.

Installation of a blade static mixer enhances the performance of SCR system due to big interaction surface area between exhaust gas flow and mixers' plates so that more ammonia and flow come in touch with each other leading to better mixing.
quality. The comparison between numerical results obtained by our model and the experimental data of Kim et al. shows that urea conversion efficiency is enhanced by 6% at an exhaust velocity of 8.3 m/s. Based on this, our SCR model proves to be effective and able to maintain a very good NOx reduction efficiency by considering the researched optimization approach.

**Keywords:** Urea-SCR, Diesel Engine, Oxides of Nitrogen, Optimization, Performance, Static Mixer, Urea conversion efficiency, UI, SAI.

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1. INTRODUCTION

Compared to gasoline engines, diesel engines have higher thermal efficiency and better fuel economy [1]. They emit less unburned or partially burned gases such as hydrocarbons (HCs) and carbon monoxide (CO) comparing to petrol engines [2]. On the other hand, Diesel engines emit higher oxides of nitrogen (NOx) and particulate matter (PM) which are considered the main species in diesel exhaust due to high combustion temperatures in the presence of excess oxygen.

NOx from diesel engine constitute nearly 90% nitric oxide (NO) while the remaining is nitrogen dioxide (NO2) [3]. Regarding marine diesel engines, Ships annually contribute to 30% of the global NOx emissions where approximately 70% of emissions occur within 400 km of land [4]. It is expected that shipping will be the single largest emitter of air pollution in Europe by 2020 [5]. Not only environment but also human health is affected by oxides of nitrogen such as respiratory system which could cause chronic lung disease.

As a result of increasing awareness of these harmful effects, international maritime organization (IMO) has issued strict limits on emissions of NOx namely Tier I, Tier II and Tier III. In order to comply with these strict requirements, different after-treatment technologies for NOx emission abatement have been introduced and SCR proved to be one of the most effective methods for marine diesel engines. This technology is mainly applicable in heavy duty diesel engines and has high NOx reduction efficiency with cost and fuel consumption efficiency. It is simple design and considered as a clean sustainable technology. Many researchers investigated the performance of SCR where the influence of injection parameters on SCR performance has been investigated by Kim et al. [6]. Spray characteristics and thermal decomposition of urea water solution (UWS) were researched in order to design a mixing chamber in SCR system of the optimal size and geometry. Jeong et al. [7] presented a numerical model for the optimal shape and location of UWS injector for SCR system in heavy duty diesel engine. They investigated the effect of injector location, injector shape and injection pressure on ammonia uniformity index and the evaporation rate of aqueous urea solution within exhaust gas tailpipe and the monolith of SCR catalyst Vikas et al. [8] investigated the influence of flow parameters on ammonia uniformity index Bacher et al. [9] investigated SCR performance over a commercial iron zeolite catalyst in a temperature range of 250 °C - 450 °C

2. NUMERICAL VALIDATION

ANSYS Fluent 15 is utilized for modeling SCR system and analyzing its performance. Exhaust gas flow is assumed to be incompressible and its motion is governed by Reynolds-
Averaged Navier-Stokes equations (RANS) which represent the conservation of mass, momentum, energy as following:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]

Mass conservation

Momentum conservation equation of X, Y and Z components respectively:

\[
\rho \frac{Du}{Dt} = \frac{\partial (-p + \tau_{xx})}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + S_{Mx}
\]

\[
\rho \frac{Dv}{Dt} = \frac{\partial (-p + \tau_{yy})}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{zy}}{\partial z} + S_{My}
\]

\[
\rho \frac{Dw}{Dt} = \frac{\partial (-p + \tau_{zz})}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + S_{Mz}
\]

Energy conservation equation

\[
\rho \frac{DE}{Dt} = -div(Pu) + \left[ \frac{\partial (ur_{xx})}{\partial x} + \frac{\partial (ur_{yx})}{\partial y} + \frac{\partial (ur_{zx})}{\partial z} + \frac{\partial (vr_{xx})}{\partial x} + \frac{\partial (vr_{yx})}{\partial y} + \frac{\partial (vr_{zx})}{\partial z} + \frac{\partial (wv_{xx})}{\partial x} + \frac{\partial (wv_{yx})}{\partial y} + \frac{\partial (wv_{zx})}{\partial z} \right] + div(k \, grad \, T) + S_{E}
\]

Transport equations for species k are also considered as following:

\[
\frac{\partial Y_k}{\partial t} + \frac{\partial (\rho u_i Y_k)}{\partial x_i} = \omega_k + \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_k}{\partial x_i} \right)
\]

2.1. Multiphase Flow Modeling

Euler-Lagrange approach is employed for modeling multi-phase flow when more than one fluid exists. Exhaust gas flow is considered as continuous phase modeled using Eulerian approach, injected particles are regarded as the dispersed phase and are modeled by applying Lagrangian approach. Discrete phase model (DPM) is utilized to describe the behavior of UWS spray. The injected particles are multicomponent and assumed to follow Rosin-Rammler diameter distribution. SST k-ω turbulence model is employed which is typically recommended as the first choice for simulating turbulent flows. It combines the advantages of both k-ε and k-ω models where the first one is used for the free stream and the other one for near wall region.

2.2. Geometry Modeling and Mesh Generation

Geometry is created in ANSYS workbench and mesh is generated in ANSA. Mesh is tetrahedral with one million cells. The domain close to the mixer is meshed using a finer mesh to properly resolve the gradients in this region as shown in figure 1 and figure 2.

Figure 1 SCR geometry created in ANSYS Workbench
2.3. Solution Methods

The pressure-based solver for steady time is used in the current work and the domain is discretized using Least Squares Cell Based. SIMPLE scheme is used for pressure velocity coupling, while Second Order Upwind Scheme is employed for spatial discretization schemes to attain more accurate results. Volume weighted mixing law is used for material density, while mass weighted mixing law is used for thermal conductivity and viscosity. KHRT model is utilized for breakup Finite-Rate/Eddy-Dissipation. Reactions are volumetric and averaging kernel nodes per cell for node based averaging is considered. Initial and boundary conditions are shown in table 1 and initial conditions of spray injection are shown in table 2.

<table>
<thead>
<tr>
<th>Item</th>
<th>Section</th>
<th>Condition and value</th>
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</thead>
<tbody>
<tr>
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<td>inlet</td>
<td>Mole fraction of exhaust gas chemical species</td>
</tr>
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<td></td>
<td>at SCR entrance: 7% v/v O2, 1% v/v H2O, 0.132</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO2, 0.0014 NO, 0.0003 NO2</td>
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<tr>
<td></td>
<td>outlet</td>
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<td></td>
<td>Turbulent Kinetic energy</td>
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<td></td>
<td>Initial temperature</td>
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<tr>
<td></td>
<td>Specific dissipation rate</td>
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<table>
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<th>Table 2 Initial conditions of spray injection</th>
</tr>
</thead>
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<tr>
<td>Spray material</td>
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<tr>
<td>Injection velocity (m/s)</td>
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<td>Cone angle (°)</td>
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<td>SMD (Rosin Rammler)</td>
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<td></td>
</tr>
<tr>
<td>Injection type</td>
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<tr>
<td>Flow mass rate</td>
</tr>
</tbody>
</table>

2.4. Optimization Approaches for SCR Performance

Two evaluation parameters are researched in terms of different injection characteristics to research the behavior of active material upstream of SCR entrance with the endeavor of developing a new evaluation parameter for SCR performance. Moreover, the effect of the static mixers on evaluation parameters is also investigated.
2.4.1. Parameters for Evaluating SCR Performance

Two estimation factors are considered for numerical study in terms of different injection characteristics as follows:

2.4.1.1. Urea conversion efficiency

It is important that SCR system can achieve a high urea to ammonia conversion which is the active material required for chemical reactions in order to obtain a high NO\textsubscript{x} reduction. Ammonia conversion efficiency is defined as the ratio of the generated mount of ammonia and the maximum amount of ammonia when urea totally decomposes and it could be expressed as following:

\[
\text{Urea conversion efficiency} = \frac{\text{Amount of ammonia generated}}{\text{maximum amount of ammonia when urea totally decomposes}}
\]

2.4.1.2. Stoichiometric Area Index (SAI)

This index is used to evaluate the distribution over SCR catalyst inlet and it is indirect measure of the mixing performance between ammonia and exhaust gas. In order to achieve high conversion over the catalyst, it is important that both NO\textsubscript{x} and NH\textsubscript{3} as the active substance are available in each monolithic channel. It is not investigated in literature and it is a good index that helps evaluating mixing development for a better understanding. SAI could be calculated based on the below formula

\[
\text{SAI} = \frac{\text{Surface area within active mole fraction}}{\text{Total surface area}} \times 100
\]

SAI is projected by highlighting the areas on the SCR catalyst inlet within the active mole fraction only, while the mole fractions outside of the acceptable span is cut out from the figures. The areas showed in such figures can be summated for the catalyst inlet and divided by the total area. This gives a single value indicating how large fraction of the inlet having a good distribution of NO and NH\textsubscript{3}. The concentration of the reducing agent with respect to NO or the NH\textsubscript{3} to NO\textsubscript{x} ratio affects the efficiency of NO\textsubscript{x} reduction in a selective catalytic reduction process. Any variation in NO conversion is not observed when NH\textsubscript{3}/NO molar ratio is in the range of 1.2–1.6. Therefore, one can conclude that NH\textsubscript{3}/NO molar ratio of 1.2 is high enough for getting a reasonable NO conversion [10]. It is used for projecting areas with the active range of NH\textsubscript{3}/NO molar ratio in the range of (0.8-1.2).

2.4.2. Effect of Injection Characteristics on evaluation parameters

The effect of two injection characteristics on evaluation parameters is measured and estimated at SCR entrance at different exhaust flow velocities. The researched injection characteristics are as following:

I. Droplet size (SMD): A common way to describe the droplet size distribution is Sauter Mean Diameter (SMD) which is defined as the ratio between the mean droplet volume and the mean droplet surface area [11]. The effect of droplet size on evaluation parameters is investigated at three different values namely 20-30 and 44 micron.

II. Injection velocity: The effect of injection velocity on evaluation parameters is researched at velocities of values 20-30 and 40 m/s.

2.4.3. Effect of Static Mixer on Evaluation Parameters

Static mixers are widely used in SCR system upstream of converter entrance in order to improve its performance. They influence flow characteristics and promotes conversion of urea into ammonia because it induces vortex flow which increases turbulence intensity that
enhances mixing between ammonia and exhaust flow. However, there is insufficient research on the relationship between flow mixing characteristics in marine engine fields. In this study, a blade static mixer is considered and installed as illustrated in figure 3 and figure 4 respectively. The blade mixer is designed as a disk with eight vanes extruded from the center which ensures good radial interaction with fluid stream. Number and direction of plates depends on the volume ratio of flow components. On the other hand, it is chosen to maintain process requirements, economics and safety simultaneously with maintaining the minimum pressure drop over the mixer.

3. RESULTS AND DISCUSSION

3.1. Effect of Injection Characteristics on Evaluation Parameters of SCR performance

The effect of the chosen injection characteristics on evaluation parameters is examined at SCR entrance at different exhaust velocities as follows:

3.1.1. Effect of Droplet Size (SMD)

Evaluation parameters are investigated at three values of droplet size namely 20, 30 and 44 micron. As evident from figure 5, urea conversion efficiency increases as SMD reduces from 44 to 20 micron. The maximum urea conversion efficiency value obtained is 44% at exhaust velocity of 8.3 m/s. At a relatively small droplet size, spray dispersibility increases which reduce evaporation time and enhance thermolysis. Smaller the droplets are, the shorter is the required vaporization time and better the droplets distribution in the flow stream. At reduced exhaust flow velocities, urea conversion efficiency is observed to increase because more residence time leads to better evaporation and higher ammonia generation. It provides a large contact area between UWS droplets and hot exhaust gas resulting in an efficient chemical reaction between NH\textsubscript{3} and NO\textsubscript{x}. The enhanced urea to ammonia conversion leads to higher NO\textsubscript{x} reduction efficiency. SAI is also observed to have the maximum value of 15.43% at droplet size of 20 micron as shown in figure 6.
3.1.2. Effect of Injection Velocity

The effect of injection velocity on evaluation parameters is investigated at 10, 20, 30, 40 and 50 m/s. It can be concluded from figure 7 that urea conversion efficiency is increased with the increment of injection velocities. It reaches its maximum value of 48% at an injection velocity of 30 m/s and it starts reducing at an injection velocity of 40 m/s. By increasing the injection velocity, spray penetration length increases and the droplet size decreases which enhance the evaporation. However, very high injection velocities lead to less urea to ammonia conversion due to incomplete evaporation because of decreased residence time and reduced inertial force. The maximum SAI value is observed to reach 16.09% obtained at same injection velocity and it starts reducing after it as shown in figure 8.

Figure 7 Effect of injection velocity on urea conversion efficiency at different exhaust velocities
3.2. Effect of Static Mixer

The results obtained show that installing a static mixer enhances SCR system performance in terms of urea conversion efficiency and SAI as depicted in figure 9 and figure 10. In case of installing a blade mixer, the obtained urea conversion efficiency is 75.1% which is 20.54% higher than the case without a static mixer. SAI has enhanced by 23.6% than the case without a static mixer.

Contours of SAI values at SCR monolith entrance at different configurations of static mixer and exhaust gas velocity are shown in figure 11. The area of the effective molar ratio of $\text{NH}_3/\text{NO}$ in noticed to become bigger when static mixers are installed and exhaust gas velocity decreases. It reaches the maximum value when both mixers are installed at exhaust velocity of 8.3 m/s.
Figure 11 Stoichiometric area index at different exhaust velocities with and without mixers

Figure 12 shows contours of NH$_3$ mass fraction through Y-direction at different configurations of the static mixer. The red-colored area represents ammonia of a high density as clear from the figure's colormap. First of all, it is noted that by installing the static mixer in cases 2, ammonia slip to the surroundings is reduced as the red-colored area at SCR outlet gets reduced which should be kept minimum. An enhancement in ammonia consumption by the catalytic chemical reaction inside converter is observed as the red-colored area gets smaller which means efficiency is promoted.

Figure 12 Contours of NH$_3$ mass fraction with and without mixers

Figure 13 and figure 14 show contours of NH$_3$ mass fraction at different cross sections between inlet and outlet of exhaust tailpipe namely $z_1$, $z_2$, $z_3$, $z_4$, $z_5$ and $z_6$. They are displayed at different configurations of blade mixer at an exhaust velocity of 8.3 m/s. It is observed that installing the static mixer induces the mixing between urea and oxides of nitrogen resulting in more generated ammonia as observed clearly in section $z_4$ downstream of mixer leading to proper effective consumption with less ammonia slip to the surroundings.

Figure 13 Contours of NH$_3$ mass fraction at different cross sections with no mixer installed
3.3. Comparison with Existing Work

The numerical results are compared with those of the experimental investigation conducted by Kim et al. [12] who researched the conversion of injected UWS to ammonia upstream of SCR monolith entrance. UWS is directly injected to the axis of the exhaust pipe at gas temperature of 673K at two average velocities namely 8.3 m/s and 10.8 m/s. The average conversion rates are measured at distances of 0.14 m, 0.21 m and 0.28 m downstream the injection point, yielding residence times between 0.01 s and 0.04 s. By comparing our model with Kim et al. model, our model with one blade mixer achieved 6% higher urea conversion efficiency at section 3 and velocity of 8.3 m/s over Kim et al. model as shown in figure 15.

![Figure 14 Contours of NH₃ mass fraction at different cross sections with blade mixer installed](image)

![Figure 15 Calculated urea conversion efficiency at different exhaust velocities at different sections compared to experimental data of Kim et al for blade mixer at 673K](image)

4. CONCLUSIONS

In this work, 3D numerical investigation on SCR performance optimization for marine diesel engine was carried out and we derived the following conclusions:

It was of great importance to numerically investigate of phenomenon taking place between injection point and SCR monolith entrance to understand the behavior of UWS spray. Evaluation parameters namely urea conversion efficiency and Stoichiometric Area Index (SAI) gave a good idea about the UWS behavior and the development of the researched process.

SAI index was an important tool to show the development of molar ratio of NH₃/NO in the effective range (0.8-1.2) in order to enhance SCR performance. Installing a static mixer positively influenced the behavior of SCR since they promoted the generation of active material (NH₃). It enhanced the evaluation parameters. Our SCR model proved to be effective and able to maintain a very good NOₓ reduction efficiency by considering the researched optimization approach.
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