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A study effects of injection pressure and wall temperature on the mixing process of NO_x and NH_3 in Selective Catalytic Reduction system

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Abstract

Diesel engines are commonly used for public transportation on-road and off-road applications. Growth production of the diesel engine is very significant from year to year. Nitride Oxide (NO_x) from diesel engine was one of the major sources of air pollution. Selective Catalytic Reduction (SCR) has been successfully used to reduce NO_x from a diesel engine with a chemical reaction from ammonia (NH_3). The mixing reaction between NO_x and NH_3 reaction can produce steam (H_2O) and Nitrogen (N_2). However, ammonia uniformity pattern usually not homogenization and the ammonia was difficult to mix with NO_x. The constant air flows incomplete to assist the spray injector to spread NH_3 to all corners of SCR. The impact study of turbulent phenomena and standard k-epsilon Low-Reynolds Number model to the mixing process in the SCR system using STARCCM+. The simulation studies are conducted under different pressure (4 to 6 bars), the injection rate (0.04 g/s) and temperature (338 K – 553 K) and the high pressure and high velocity magnitude creating turbulent swirl flow. The ammonia decomposition process and mixing process with NO_x were investigated using a box with optical access. The simulation and numerical study results validated using back pressure value and the distribution of NO_x concentration value from the catalyst outlet. The wall temperature will increase the urea evaporation to generate ammonia and gas pressure will increase the mixing process and chemical process in the SCR system. These reactions enable to optimize the SCR system technology which eventually able to reduce the NO_x quantity from a diesel engine.

Keywords: diesel engine; wall temperature; wall impingement; urea water solution (UWS); urea injection; selective catalytic reduction (SCR).

I. Introduction

Diesel engines are commonly used for public transportation on-road and off-road applications. Growth production of the diesel engine is very significant year to year [1]. The diesel engine is used for commercial and passenger vehicle [2][3][4]. Some of the major advantages of diesel engine over another fuel engine are the higher durability and increased fuel efficiency. On the other hand, the main disadvantage is related to exhaust emissions from the diesel combustion process. The emission of the diesel engine is one of the major sources of air pollution which need to be controlled by the after-treatment system. Government has released a regulation for automotive industry related to the exhaust gas emission to further reducing the nitrogen oxide emissions.

The emission rules have reached the pollution limit of the EURO VI and the US TIER 2 regulation [1][5][6]. The ammonia in the Selective Catalytic Reduction (SCR) as the main solution to control specific emissions from the engine. The technology of SCR used the injection of a urea liquid into the exhaust system. The hot temperature from exhaust makes a urea-water solution (UWS) evaporates and decomposes to be ammonia. Ammonia concentrate used as reducing nitrogen oxides (NO_x) in the SCR system.

Many researchers study around the injector for spraying urea (NH_3), gas temperature, and catalyst

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substrate in the SCR system, but the ammonia still difficult to mix with NO_x. Based on our previous study [7], it has been mentioned that the urea is difficult to evaporate and easily attached to the wall and making the solid deposit in the system. It is consistent with the study carried out by Hasan [8] which found the solid deposited effect to the mixing process at the SCR system.

The most important concept for the mixing process is the turbulent airflow from the exhaust gas in the SCR system. Exhaust airflow was assisting the spray injector to spread NH_3 to all corners in the SCR system. To solve that situation, this study presents a simulation and experimental study of the turbulent phenomena impact and the standard k-epsilon Low-Reynolds Number model to mixing process in the SCR system using STARCCM+. To create turbulent in the SCR system, this study uses pressure from the exhaust gas and wall temperature from the SCR system.

The simulations study based on the exhaust gas system with a high pressure to create turbulent swirl flow. The ammonia decomposition process and mixing process with NO_x were investigated using a box with optical access. The data obtained from the optical box can assist the identification of the actual condition in the SCR system. The effects of wall impingement on deposit formation in diesel SCR system has been investigated the wall temperature (338 K) and (573 K). In the previous research carried out by Auvray [9], it was shown the temperature (473 K) and (598 K) can be used to analyze kinetic modelling on NH_3 in the SCR system.

Furthermore, our previous study [4] also used a high temperature of 536 K to study the ammonia uniformity in SCR system technology. A similar study from Smith [2], it has used a low temperature of 473 K and a high temperature of 608 K for analyzing the deposit formation reaction. Based on those investigations, the temperatures used in this system are 338 K for low wall temperature and 553 K for high wall temperature. The simulation and numerical study results validated using back pressure value and the distribution of NO_x concentration at the SCR system.

II. Materials and Methods

A. Mathematical model

The numerical study with 3D simulation for understanding the mixing process in the SCR system was shown with STARCCM+ software version 11.04. In another paper from Fischer *et al.* [10], compare the Reynolds-averaged k-epsilon-models and Reynolds-stress-model (RSM) to accounting the anisotropic character of turbulence in the swirl flow. Fischer *et al* used pipe with oval/flat crosses section for assist mixing process in the SCR system. The RSM describe the anisotropic turbulence between the primary swirl core and the outer secondary. This method is useful for understanding the TKE values in the pipe cross section and dissipation value in the swirl core. However, the RSM difficult to predict the highly turbulent reaction at the inner and outer swirl core.

Yi [11] has analyzed the ammonia homogenization from two different mixers with renormalizing of Navier-Stokes equations (RNG) and the k-epsilon model for turbulence study. The computational fluid dynamic (CFD) model of their research simple SCR system installation. The straight pipe with urea injector and leading into the catalyst. The urea injector is located at the wall with a 90° angle relative to the main flow. Without a mixer system, the low quality of ammonia uniformity has resulted. Integrating a helix swirl mixer in the system leads the ammonia to raise the good quality of uniformity.

This study was applying straight pipe and optical box with fully SCR system. The urea injector is located at top of the optical box. That urea can release the UWS spray was from top to bottom. This observed is focus on the distribution of exhaust gas with pressure to get the turbulence quality without the mixer. The eddy viscosity from the k-epsilon equation, determined from a single turbulence length. The calculation of turbulent diffusion can achieve by the specified scale. Although in the real system, all motion scales will contribute to the turbulent diffusion.

The numerical computation with a realizable k-epsilon model for resolved the viscous layers and viscous sublayer in the SCR system. These equation functions of wall treatment can be extended and solving the multiphase flow phenomena and motion of gasses from NO_x and ammonia wherein the gasses is characterized by properties that are aggregated over a large number of individual molecules [12][13]. Each particle in the system has associated with a physical equation, such as density, velocity, vorticity and temperature. The vector quantity in the numerical properties assumed to be observable and hence there are 'streamlines' at the local velocity vector. Streamlines can never cross except at point sources or sinks of fluid. The transport equations for the Low-Reynolds Number with k-epsilon model equation can solve the computational domain:

$$\frac{d}{dt}\int_A \rho\varepsilon \, dV + \int_A \rho\varepsilon(v - v_g).da = \int_A \left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon.da + \int_V \frac{1}{T}\left[C_{\varepsilon l}(G_k + G_{nl} + C_{\varepsilon 3}G_b) - C_\varepsilon 2\rho(\varepsilon - \varepsilon_0) + \rho\gamma_y + S_\varepsilon\right]dV \quad (1)$$

where S_k and S_ε are specified source properties, ε_0 is the ambient turbulence value for turbulence decay counteracting, ρ is the source density, and G' is the additional product from source term that is given by:

$$G' = Df_2\left(G_k + 2\mu\frac{k}{d^2}\right)\exp\left(-ERe_d^2\right) \quad (2)$$

where D is the distance to the nearest wall of the source terms, d is the distance to the wall, k is turbulent kinetic energy, μ is dynamic viscosity, and f_2 is a damping function that is defined as:

$$f_2 = 1 - C\exp(-Re_t^2) \quad (3)$$

where

$$Re_d = \frac{\sqrt{k}d}{v} \quad (4)$$

and

$$Re_t = \frac{k^2}{\varepsilon v} \quad (5)$$

The coefficients C and E are using the default values of 0.3 and 0.00375. and the value for coefficient D in the system is in Equation (6):

$$D = \frac{C_{\varepsilon 2}}{C_{\varepsilon l}} \approx 1.3 \quad (6)$$

However, direct numerical simulation (DNS) of low-Reynolds number channel flow suggests that better results are obtained with $D = 1$, which is the default value that is used in STARCCM+. DNS was the presence of free stream turbulence, inaccuracy computing method the $D = 1$ was used for minimizing the error result from turbulence equation. The momentum coupling model for flow sections used the vertices scale, the turbulent viscosity μ_t has a relation on getting the turbulent kinetic energy k and dissipation ε, in equation (7):

$$\mu_t \sim \frac{k^2}{\varepsilon} \quad (7)$$

With regards to the scalar transport model equation, a direct proportionality of turbulent diffusive momentum and scalar transfer is assumed. This method can explain the turbulent scalar diffusion is directly linked to the turbulence models viscosity prediction in Equation (8):

$$\rho \mu_J \gamma = -\frac{\mu_t}{Sc_t}\frac{\partial y}{\partial x_J} \quad (8)$$

The constant equation to get the proportionality value is used the turbulent Schmidt number Sc_t. An underestimated turbulent viscosity value in the equation model can be stable by reducing the Schmidt number value (0.7 – 0.9). Throughout the following investigations by Wardana [7], the turbulent Schmidt number for Standard k-epsilon Low-Reynolds Number model used the default value of 1.0 for described in this literature review.

1) Thermolysis and evaporation of UWS droplets

Despite numerous experimental studies have been conducted [4][14][15], theoretical understanding for the decomposition and evaporation of UWS and Adblue droplets are still not fully investigated. A theoretical study [9][12] was implemented using STARCCM+ for simulation which then compared by experimental works to get the best accuracy. This method assumes two processes of the UWS evaporation until the UWS droplet is only composed of urea. It uses a spherical method for the evaporation and decomposition processes without using urea crystallization in the process.

Rapid mixing model is used to evaluate the dissolved urea on the evaporation process of urea water solution. Because this model can identify the high transport coefficients from the liquid phase. The result can explain the homogenous distribution temperature in the system, concentration particle value and fluid properties in the UWS droplet [9]. The variation model in UWS concentration droplet's can be evaluated by Equation (9):

$$\frac{dY_u}{dt} = -\frac{m_{vap}}{m_d} Y_u \quad (9)$$

where m_d is the mass of droplet particle, dY_u is urea concentration value and m_{vap} is a vapour value of mass flow in the system. The evaporation rates in this equation are calculated by the Abramzon-Sirignano model [12]. That model useful for low computational to observe the UWS droplet particle and suitable predict the spray modelling [12]. The urea particle will easily melt at 400 K [12] and the Arrhenius model can describe that chemical kinetics reaction by Equation (10):

$$\frac{dY_u}{dt} = -A_f S \exp\left(-\frac{E_a}{RT_d}\right) \quad (10)$$

where S is droplet surface area in the system, A_f is the frequency factor [kg/(sm^2)], R is the universal value, T_d is the droplet temperature for gas constant and E_a is the activation of energy in the system.

2) Urea water solution injection

Urea-water solution is the most commonly used for ammonia precursor in the SCR system because this material was safe for the environment. The commercial name for UWS was Adblue, this aqueous was a combination from 67.5 to 70 % deionized water and 30 to 32.5 % urea [12]. Gas emission from diesel engine usually produces more than 90 % of NO_x and 5 to 10 % of NO_2. That quantity depending on the diesel engine type. NO_2 from diesel engine emission is useful for fast SCR reaction process. That chemical is produced from engine-emitted NO when oxidation reaction in the catalyst.

In order to describe the UWS injection phenomena in the SCR systems, this study used a mathematical description to explain all processes [3][9][12]:

- Interaction momentum between Exhaust gas and UWS droplets
- Thermolysis and Evaporation of UWS droplets
- Heat transfer from exhaust temperature to the wall and droplets. This section presents the mathematical basics model to implement the CFD modelling conduct the numerical simulations of the SCR system by STRACCM+ software. The flowchart model for this simulation is shown in Figure 1.

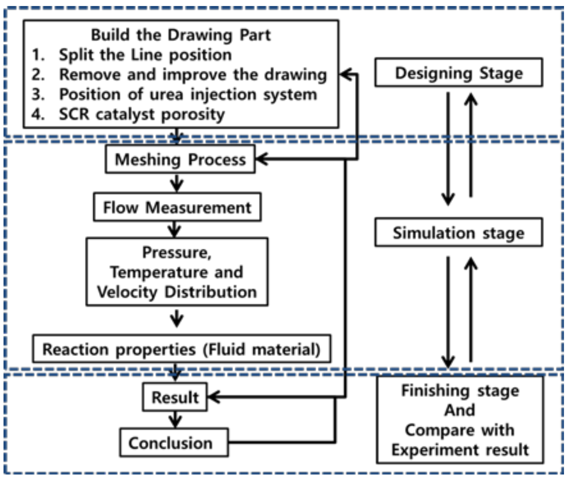

Figure 1. The flowchart of simulation process

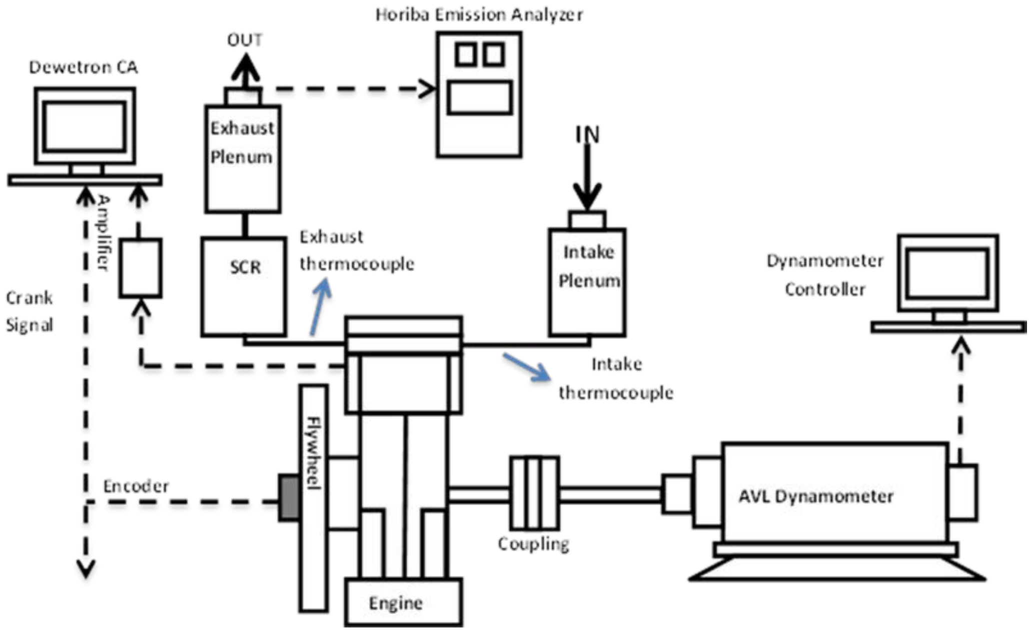

Figure 2. Schematic diagram of test engine and measurement setup

B. Experimental setup

The experiment condition used a single cylinder with 498 cm^3 of displacement, naturally aspirated engine with 4-cycle, and SOHC 4 valves system to get the precision of the engine test. The engine specification is shown in Table 1. The pressure at the exhaust was 4 to 6 bar [5][6][16] and leading into the optical box with straight pipe. A schematic diagram for the optical box test is shown in Figure 2.

The pressure from UWS injector was ranging from 4 to 6 bar, the ammonia injection rate (0.04 g/s) and exhaust temperature constant in 338 K – 553 K [5][6][16]. The injection specification is presented in Table 2. The optical box for measuring position and dimension was realized with silica glass. The positions and dimension were chosen to minimize the effect of the gas flow in the system. The optical box gas flow distribution is shown in Figure 3. The mixing process between NO_x and ammonia is observed in the optical box. The Horiba MEXA-7100DEGR is used to identify the emissions value from the system (hydrocarbon and NO_x).

Table 1.
Engine specification

Engine parameter	Value
Displacement	498 cm^3
Bore	83 mm
Stroke	92 mm
Compression ratio	19.5
Con. rod length	145.8 mm
Crank radius	43.74 mm
Valve system	SOHC 4 valve
Fuel system	Electronic common rail

Table 2.
Ammonia and exhaust injection

Parameter	Value
Exhaust inlet	10, 15, 20 m/s
Injector inlet	10, 15 m/s
Injection rate	0.04 g/s
Temperature	338 K – 553 K
Pressure	4, 5, 6 bar

C. Validation of simulation

To verify the Standard k-epsilon Low-Reynolds Number model simulation results from STARCCM+, the observation from ammonia uniformity at the SCR system have been carried out on the experiment test [5][17]. The exhaust line directly connects with the SCR system. The Horiba MEXA-7100DEGR can determine the gas distribution and the hydrocarbon value from the catalyst outlet.

The Standard k-epsilon Low-Reynolds Number equation model is suitable for computing the convection flows. The situations to have a Low-Reynolds Number version of the Standard k-epsilon model, and Non-linear Constitutive Model as shown in Table 3.

The setups have two-equation models for the simulation of the measured ammonia uniformity. The error value for the velocity magnitude model is a good agreement to observe the validated literature cases for the k-epsilon model in the SCR system simulation [2][11]. By considering the complete process from UWS spray to the ammonia distribution in the optical box.

Table 3.
Analyzed turbulence models and boundary conditions

Setup	Turbulance model	Boundary condition [a]
1	Standard Low Reynold Number k-epsilon	PI - VO

[a]V = Velocity; P = Pressure; I = Inlet; O = Outlet

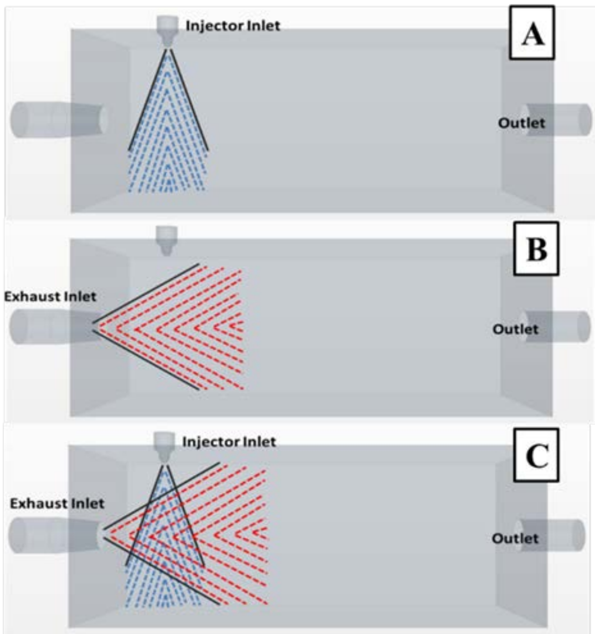

Figure 3. The measurement position of exhaust flow and ammonia injector spraying to the optical box: (a) Urea injection spray pattern; (b) Exhaust gas pattern; (c) Combination pattern from urea and exhaust gas

III. Results and Discussions

A. Exhaust simulation gas

Simulated distribution of the exhaust pressure streamlines in an optical box system, as it has been predicted by STARCCM+. This simulation using the Standard k-epsilon Low-Reynolds Number model with the prediction on the effect of exhaust gas for ammonia decomposition phenomena can be calculated with the Schmidt number value. This energy value used to determine the turbulent viscosity and diffusion constant in the equation model. Besides that, this simulation model is implying the reduction of the anisotropic information for turbulent energy quantity at least for the scalar transport value.

Figure 4 shows the difference turbulence streamline and scalar distribution in the optical box. Gas flow in the optical box is the most important indicator to mix ammonia and NO_x. This flow strongly influences the homogenization of ammonia vapour, even without a sufficient temperature from

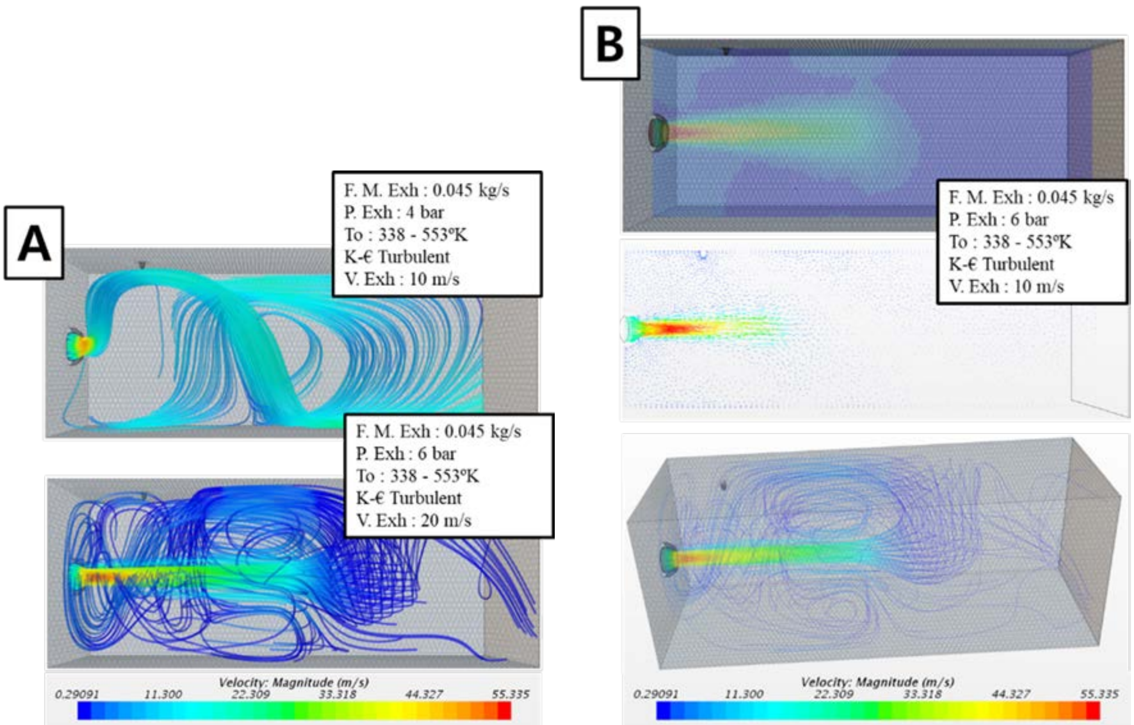

Figure 4. The difference turbulence streamline and scalar distribution in the optical box: (A) Exhaust turbulent phenomena and (B) Exhaust scalar phenomena

the ammonia injection. The amount of pressure for mixing process of NO_x and ammonia is shown in Figure 4(A). This picture described a pressure ratio between the lowest (4 bar) and the highest (6 bar). The colour line explains the velocity value in the simulation. However, the quality of the mixing process from Figure 4 was explained by the quantity of gas distribution in the simulation. It affects the different movement of air in the optical box. When the higher pressure was used, this condition makes the more diffuse flow of air generated and it was a good result for mixing ammonia and NO_x. But instead, when the smallest pressure is used, ammonia and NO_x mixing is difficult to be created as airflow having difficulties to spread close to the wall and makes ammonia on the wall could not be parsed by airflow.

The airflow and pressure quantity also increasing the wall temperature value in the optical box. Figure 4(B) explains the temperature distribution in the simulation. Heating wall temperature propagates by flowing heat of exhaust gas from inlet to the outlet, more high gas flows from the exhausts more heat of the wall temperature, and its effects on the reduction ammonia droplet in the wall. This statement also has been explained in our previous study [7] which is observed the wall temperature value for predict the urea injection process in the SCR system. Figure 5 shows the velocity magnitude quality. As can be seen from the figure, the constant exhaust flow mass value achieve at 0.045 kg/s, the maximal flow mass value achieve at 3.15 kg/s and minimal flow mass at -3.5 kg/s in the optical box. The free gas at the optical box makes flow mass in an optical box unstable in the first time. Flow mass is difficult to spared before free gas come out from the optical box. That case also happens in constant velocity magnitude. Maximal velocity occurred due to the empty condition when the exhaust gas inside the optical box.

Figure 6 shows the pressure and force value. As can be seen from Figure 6, constant pressure occurred in 20 s after the exhaust come from the inlet. An empty condition in the optical box makes pressure decrease significantly to -102.15 bar. Exhaust gas occupies empty space in the optical box to encourage the free gas came out from outlet to generate exhaust force gas and make pressure increase constantly after declining. Maximal pressure happens in 13.2 bar and decrease after 12 s exhaust came from the inlet. That was contradicted with exhaust gas force value when the exhaust gas pressure value decreases in an optical box, exhaust gas forces increase until 19.78 kN and the force value decrease on -2.63 kN. Massive pressure was counted by volume of the optical box, the extent of affecting the increase and decrease of the exhaust gas pressure against time. With a dimension of 90 x 30 x 30 cm^3 of the optical box, the exhaust pressure needs 20 s for stabilizing into 1 bar. If using the small volume that can easily stable lowest than this simulation.

B. Injector effect on exhaust simulation gas

The distribution of the exhaust pressure can predict the streamline reaction in the optical box. At

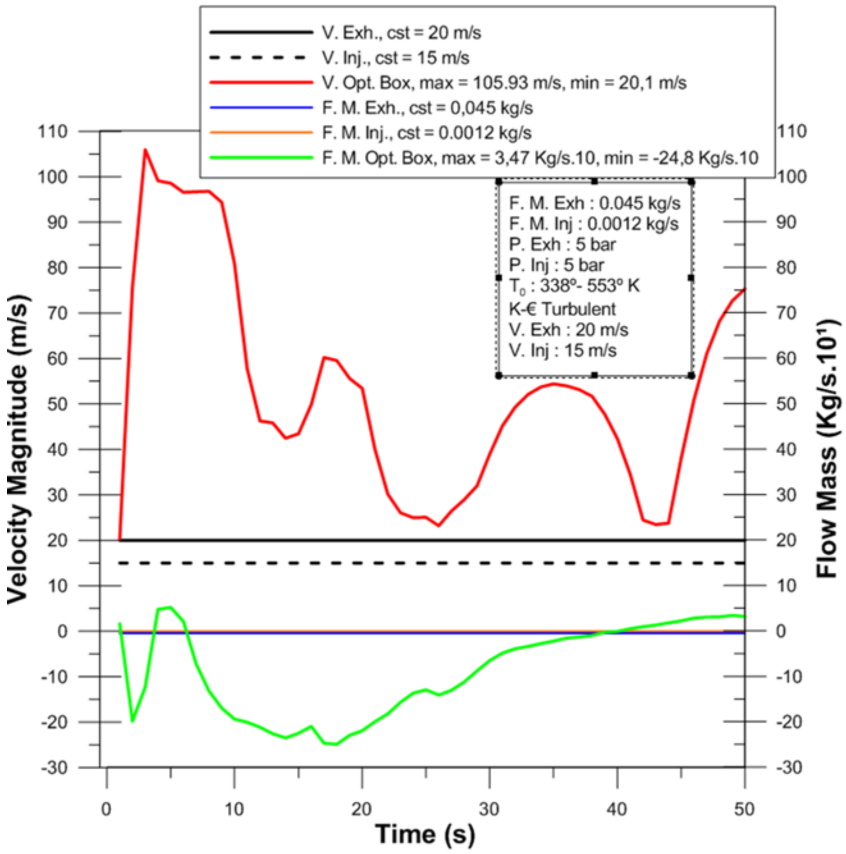

Figure 5. Velocity and flow mass effect at the optical box

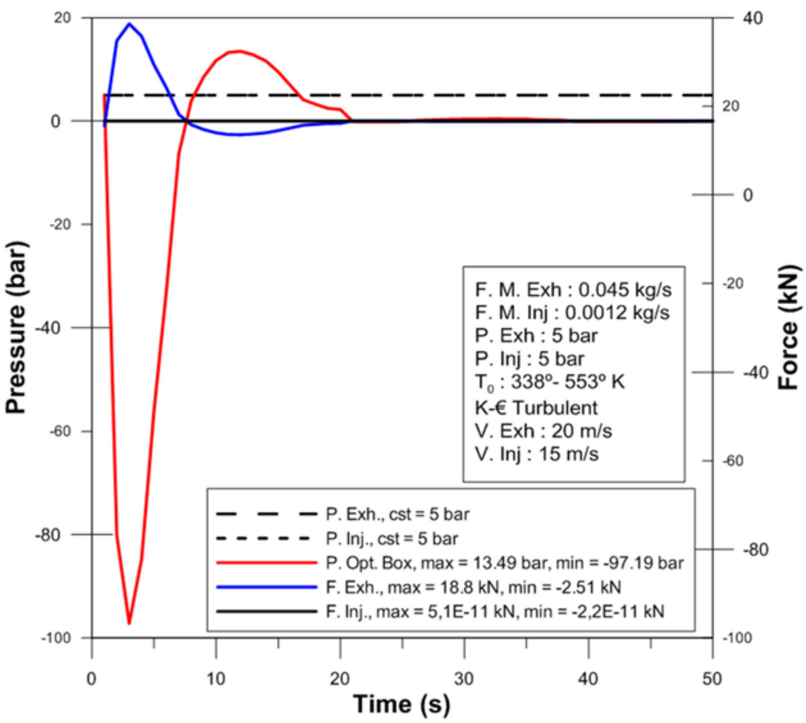

Figure 6. Pressure and force effect at the optical box

the first step of the exhaust inside the optical box, the pressure of exhaust was dropped to -102.15 bar, that condition also happen in the real SCR in public vehicles. The amount of the pressure drop was depending on the size of the exhaust muffler (pipe and SCR system). When the SCR system has a pressure drop, the exhaust flow is difficult to spear the adblue from urea injector. The urea from adblue attached in the wall will settle and harden because the wall will heat up due to the creeping temperature of the engine heat. That reaction has an effect after long period application of SCR system in the diesel engine.

The timing for spraying adblue in commercial diesel engine has been analyzed in exhaust simulation gas. For injector condition, the constant pressure and velocity value can set the turbulent flow in the system. The distribution of gas and liquid were accounted, but it does not give an insignificant impact from the spray characteristic in the flow field. That reaction occurring because the injector has low pressure and momentum for spraying the UWS. Nonetheless, the flow field during the transient condition keeps valid.

Figure 7 shows the difference turbulence streamline from UWS injector and exhaust gas in the optical box. This simulation shows that the NO_x and ammonia mixing can be observed and analyzed in the optical box. Nonetheless, interdependencies from the liquid and gas phase with swirl fan mixing are avoided in this study. The ammonia vapour concentrations got the averaged value by each computational cell when one-time injection duration. The resulting quasi-steady spatial for ammonia distributions value is observed on the cross sections as long as in the steady flow quantities. The simulation was plausible with visualizing and evaluates the ammonia homogenization process in the optical box.

The turbulent kinetic energy (TKE) is the main parameter to determine turbulent viscosity and turbulent diffusion in this simulation [5]. Figure 8 shows the TKE value on the optical box. This TKE result got the maximum curves when the exhaust gas comes to the inlet (2.5 s). The gas flow distribution creating the steep velocity gradients by the source of turbulence.

The kinetic energy structure divided into small-scale structures turbulence energy and transferred into dissipates rate of energy. The turbulent dissipation value in the system is shown in Figure 7. Though just using the k-epsilon model, the turbulent scheme showed very clearly. Beside that for detail result, it still needs more deeply parameter using deference mathematic model.

C. k-epsilon model validation

The ammonia uniformity in this study resulted that without a mixer system, the low quality of ammonia uniformity has resulted. Integrating a helix swirl mixer in the system leads the ammonia to raise the good quality of uniformity. That result is explained on this validation purposes [10]. 2 results from this study will be compared to find the best values by the Standard k-epsilon Low-Reynolds Number model [10].

Figure 9 shows the back pressure value between simulation and experiment in the optical box. This result explains the mass flow quantity from exhaust temperature and the amount of gas distribution. The Standard k-epsilon Low-Reynolds Number model has been calculated by heat temperature from exhaust inlet with the increasing wall temperature parameter. In that case, the temperature was the

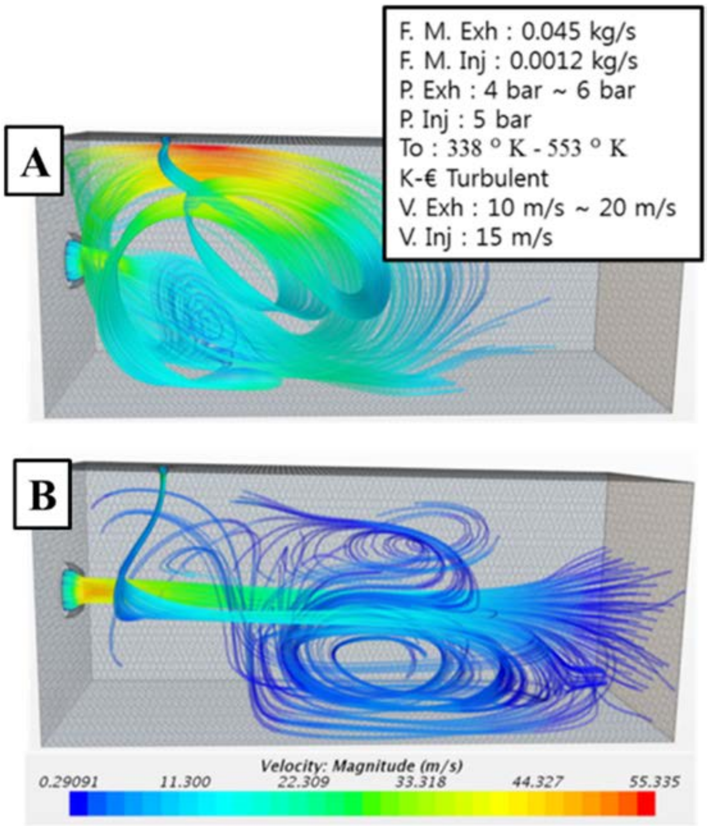

Figure 7. Exhaust and injector turbulent phenomena of (A) with low exhaust pressure and (B) with high exhaust pressure

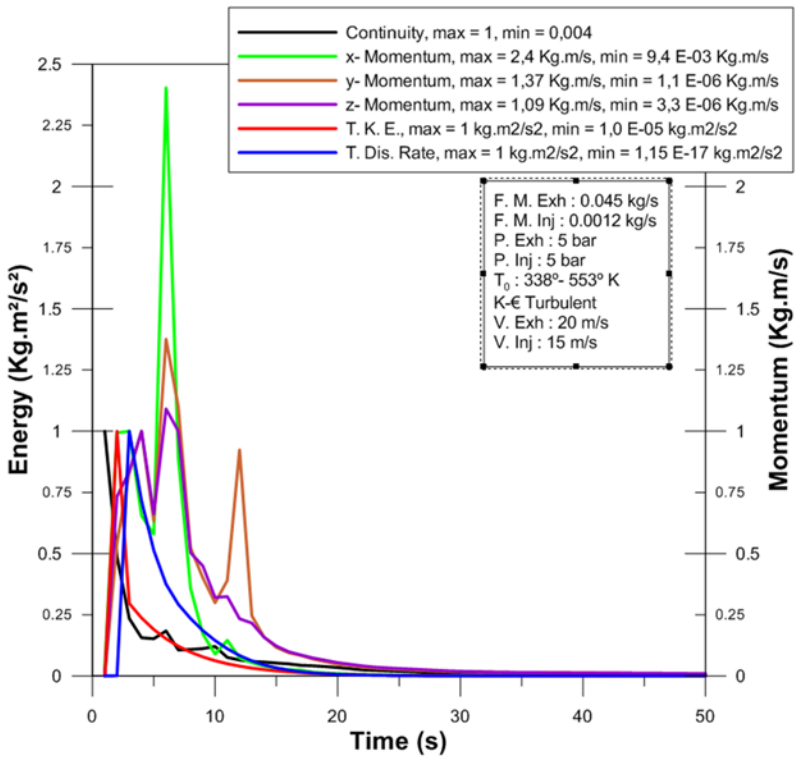

Figure 8. Turbulent kinetic energy (TKE) and turbulent dissipation rate (TDS) effect in optical box

most decisive to mix ammonia and NO_x, besides the turbulence in the optical box. The back pressures value occurring at low volume condition can determine the magnitude of measurement precision.

This parameter condition useful for computation in the validation discussion. The particular range in this simulation has offset value of approximately 1.0 bar and that value better 0.2 bar from RSM simulation condition. The measuring value for back pressure at high volume flow occurs when the measurement has precise and reliable data [10]. That parameter can predict simulation by comparing the

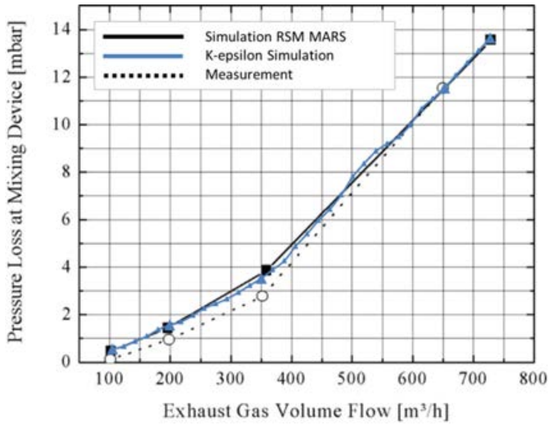

Figure 9. Comparison pressure loss at mixing device

different turbulent model, which is expected to get similarities and accuracy data measurement and simulation.

IV. Conclusion

Simulated distribution of the exhaust pressure streamlines in the optical box system, as it has been predicted by STARCCM+. Gas flow in the optical box is the most important indicator to mix ammonia and NO_x. This flow strongly influences the homogenization of ammonia vapour, even without using a sufficient temperature from ammonia injection. Heating wall temperature propagates by flowing heat of exhaust gas from inlet to the outlet, more high gas flow from exhausts more heat the wall temperature, and the effect on the reduction ammonia droplet in the wall. The free gas at the optical box makes a mass flow in the optical box unstable in the first time. With a dimension of 90 x 30 x 30 cm^3 of the optical box, the exhaust pressure needs 20 s for stabilizing into 1 bar. If using the small volume that can easily stable lowest than this simulation. An empty condition in the optical box makes the pressure decrease so deeply until -102.15 bar when exhaust came from the inlet. Massive pressure was counted by volume of the optical box used, the extent of affecting the increase and decrease of the exhaust gas pressure against time. For injector condition, the constant pressure and velocity value can set the turbulent flow in the system. The distribution of gas and liquid were accounted, but it does not give an insignificant impact from the spray characteristic in the flow field. That reaction occurring because the injector has low pressure and momentum for spraying the UWS. Nonetheless, the flow field during the transient condition keeps valid. The turbulent kinetic energy (TKE) is the main parameter to determine turbulent viscosity and turbulent diffusion in this simulation. In comparison TKE curves and TDS curve, the result has a different path to describe the turbulent energy based on the region section. The high momentum in this result can validate the strong energy from the exhaust to increase the distribution of ammonia in the system. Although this study has different parameter and CFD models with others study, this result can be good knowledge for the researcher to understand the mixing process of ammonia and NO_x in SCR system technology.

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Nomenclature

CFD : Computational Fluid Dynamic
MARS : Monotone Advection and Reconstruction Scheme
NO_x : Nitrogen Oxide
K : Kelvin temperature scale
SCR : Selective Catalyst Reduction
TKE : Turbulent Kinetic Energy
TDS : Turbulent Dissipation Rate
UWS : Urea Water Solution
RSM : Reynolds Stress Model

Declarations

Author contribution

M.K.A. Wardana as the main contributor of this paper. All authors read and approved the final paper.

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Conflict of interest

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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