ABSTRACT: SCR systems are mainly used in exhaust systems as an emission control device for diesel engines with excellent thermal efficiency. In this paper we explored the design of mixing devices which are an important element in the system. The optimum shape for various conditions and designs to disperse ammonia from a urea solution was optimized with CAE and design space exploration, and validated with visualization experiments for correlation.

KEY WORDS: Heat engine, Post treatment system, Numerical calculation, Urea-SCR system, Mixer, Optimized design [A1]

1. Introduction

With the advances at diesel engine efficiency and demands for fuel economy, urea selective catalytic reduction (Urea-SCR) system with mixer and the dosing systems become important devices to achieve the emission regulation targets. For a given exhaust environment, injecting the precise amount of diesel exhaust fluid (DEF), fully decomposing it into ammonia and uniform mixing with the exhaust gas is very critical. To facilitate the evaporation and mixing of urea solution within the excellent performance, careful examination should be required for optimum mixer and dosing system devices. In this paper, we described the optimized shape of the mixer with various design variables and constraints by implementing the computational fluid dynamics (CFD) and an optimization software. As a result, one of the optimized mixing system design by numerical analysis confirmed with the experimental study.

Diesel engines firstly developed to compete with the steam engines, which designed to move very heavy loads, generating high torque and constant speed. With advanced technological development at diesel engines, now they have the highest thermal efficiency of any other internal combustion engines with a smaller volume of fuel to perform a specific amount of work. With this advantage of diesel engines, they mainly used in passenger cars in Europe, submarines, ships, locomotives, trucks, and off-road vehicles.

Diesel engines produce less carbon dioxide (CO₂) than a comparable gasoline engine yet emit more regulated pollutants, including oxides of nitrogen (NOₓ), particulate matter (PM), and hydrocarbons (HC). Urea-SCR technology is one of the promising technology used in diesel engine applications. In Urea-SCR system, the mixing of the sprayed DEF in the exhaust gas must evaporate and decompose to ammonia adequately prior to the SCR catalyst inlet (1). For some applications, there is no enough length for sufficient mixing because of layout restrictions. Urea mixers, in such cases are very critical to improve the flow mixing by creating turbulent flow and enhance the DEF evaporation. When developing such urea mixers, some performance criteria conditions must be evaluated mainly including NOₓ reduction efficiency, uniformity at SCR catalyst inlet, and low-pressure drop.

2. Mixer Design Approach

Zheng et al. (2) represented a development cycle, which is an iterative loop for urea mixer design as in Fig.1. In this development cycle, if the design concept satisfies the performance criteria with CFD results, the development forwards to the next level of prototypes and flow lab tests. With the successful flow performance, cycle forwards to the deposit and durability tests. When the current design does not meet the criteria, it returns to first cycle with some tuning or a new design concept.

![Fig. 1 Mixer development cycle](2)
One of the mixer type developed within the development cycle is a two-stage mixer as shown in Fig. 2 (3).

3. CAE Analysis Model

3.1. Model Configuration

In this study, an analysis model is considered with pipes, urea-injector, and a type of two-stage mixer (see Fig. 3). Three-dimensional CFD analysis is performed to understand the mixing performance of the two-stage mixer by looking at the uniformity index and spray flow distribution.

The exhaust gas is assumed to be air. Air Inlet is defined as a mass flow rate inlet where the mass flow and the temperature are shown in Table 1.

| Air | Injection Water |
|-----|-----------------|
| Mass Flow [kg/h] | 173 | 20 |
| Temperature [°C] | 20 | 0.22 |
| Mass Flow [g/s] | 20 |
| Temperature [°C] | 46,357 |

Water is injected into the airflow through one nozzle as DEF for correlation with experimental study. The outlet is specified to a pressure outlet and the pipe walls are defined as adiabatic condition.

The volume mesh generated for this analysis is shown in Fig. 4 with 2,194,219 cells including prism layer and polyhedral. For inlet and outlet pipe mesh extruder function is used to develop a uniform velocity profile and enhancing of convergence. Two prism layers are used near walls to resolve the flow separation. The mesh refinement applied at the region close to the mixer.

3.2. Governing Equations

In this study, the steady-state Eulerian-Lagrangian Multiphase CFD analysis has been performed for the calculation condition. The physics continuum is a continuous phase whose governing equations are expressed in Eulerian form. For solving the pressure and velocity field, we used the segregated flow solver which is a Rhie-and-Chow-type pressure-velocity coupling method combined with a SIMPLE-type algorithm. The Lagrangian Multiphase model permits solving an arbitrary number of dispersed phases, each modeled in a Lagrangian framework.

For continuous Eulerian framework Reynolds-Averaged Navier-Stokes equation is solved with the Realizable k-ε turbulence model (4) with the two-layer approach. In this model the turbulent viscosity is computed as

\[ \mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \]

where \( C_{\mu} \) is no longer constant as with the standard \( k-\varepsilon \) model, variable determined from an equation (4). The model coefficients are defined as

\[ C_{K} = \max(0.43, \frac{\eta}{5+\eta}) \quad \text{where} \quad \eta = \frac{Sk}{\varepsilon} \]

The other coefficients in the model are \( C_{\varepsilon} = 1.9 \), \( \sigma_{K} = 1.0 \) and \( \sigma_{\varepsilon} = 1.2 \)

Injected water spray is modeled by tracking the individual droplets with Lagrangian approach. The conservation equation of momentum for a droplet mass particle is given as follows (4)

\[ \frac{d}{dt} \frac{m_d}{V_d} = F_d + F_b \]

\( F_d \) represents the forces acting on the surface of the particle, and \( F_b \) the body forces.

\[ F_d = F_d + F_p + F_v \]

\( F_d \) is the drag force, \( F_p \) is the pressure gradient force, \( F_v \) is the virtual mass force.
Air on the droplet will be much smaller since the density of the water is much larger than the air density. So the body forces $F_B$ are neglected in this calculation. The droplet mass particle trajectory equation is defined as

$$\frac{dx_d}{dt} = V_d - V_g$$  (5)

where $x_d$ is the position of the droplet particle, $V_d$ is the particle velocity, and $V_g$ is the grid velocity.

Turbulence dispersion model which is defined by Gosman and Ioannides (5) is activated to interact the injected droplets with the individual turbulent eddies from the flow. Injector initial droplet diameters are defined by the PDPA data of the injector. For the droplet breakup, two different models are defined (6,7). The quasi-steady single-component droplet evaporation model (8) is applied for injected water evaporation. This model assumes droplets are internally homogeneous, consisting of a single liquid component.

3.3. Analysis Results

Uniformity index (UI) of evaporated water and flow on a cross section plane surface at 150mm (see Fig. 5) far distance from the mixer is used as the mixing performance of the system. The uniformity index $\gamma$ is computed on the surface as

$$\gamma = 1 - \frac{\sum|\bar{\phi} - \bar{\phi}|A_f}{2|\bar{\phi}|\sum A_f}$$  (6)

where $\bar{\phi}$ is the surface average of $\phi$, $\phi_f$ is the face value of the selected scalar and $A_f$ is the area of the face. If the selected scalar distribute equally, the resulting number of uniformity index is 1.0.

Pressure drop of 104 Pa is occurred between the inlet and outlet of mixer. Figure 5 shows the distribution of flow and vapor at the specified cross section. Two-stage mixer shows very high mixing performance for both flow and vapor even at a very short mixing length.

4. Experimental Study

4.1. Test Specifications

For confirmation and correlation of previous analysis model, at first we checked the visualization experiment methods (9). Then we established the experimental system. The system includes the acrylic pipes, two-stage mixer, air junction part, ultrasonic air flowmeter (Aichi Tokei TRX65D-C/4P), 1-hole injector and dosing system (Tenneco XNOx LFE6), high speed camera (NAC HX-5), standard video camera (Sony HDR-CX485), sheet lasers (KATO KOKEN G450 0.45W and 2W) and two blowers (Bosch GBL800E). The overall test setup is illustrated in Fig. 7. In addition, Fig. 8 shows the mixer visualization setup for spray flow distribution. Figure 9 shows the setup for visualization of water distribution at the cross section. Airflow rate is adjusted with one blower and ultrasonic air flowmeter. Water is injected instead of DEF for correlation with analysis model. Operating condition is set same as in Table 1.
Spray flow distributions were recorded with high speed camera frame rate of 30,000fps, shutter speed of 100k. Water distribution at specified pipe cross section was recorded with 10,000fps, shutter speed open.

4.2. Test Results

Figure 10 shows the visualization of spray flow with a zoomed view at mixer blades. The spray flow hits mainly to the lowest long blade, and partially hit above two blades because of low mass flow and low temperature condition. Residual water distribution at cross section 150 mm behind mixer can be seen in Fig. 11. It explains the evaporation process is not completely finished by 100 percent, which give very important performance information about the vapor uniformity.

4.3. Correlation with CAE Analysis Model

Visualized spray distribution in Fig.12 (a) is compared with analysis result by sketching the spray traction outlines on the test result. It was confirmed that the spray characteristic is well correlated with CAE model. Again, borderlines of vapor concentrations at Fig. 13 (b) are sketched into Fig. 13(a) (image processed of Fig. 11). The region that the water droplets are exist means that the vapor concentrations are lower at that region. Water droplets detected at region outer of these borderlines have almost similar pattern with CAE model.

5. Design Exploration of Mixer Shape

5.1. Methodology

We confirmed current design performance with the visualization experiment in previous sections. For more improvements at mixing performance, still we need some design concept optimization. Therefore, we adopted a design space exploration tool for optimization of mixer and injector design concept. For the design space exploration, there are several type of optimization methods. In this study a new simulation tool, HEEDS provided by Siemens PLM software was used. Key advantage of HEEDS is its proprietary search algorithm, SHERPA, which is a hybrid and adaptive search framework and automatically adapts to the design space by blending and leveraging various types of search strategies, such as global and local algorithms. Because of its adaptive nature, the user only needs to set the number of function evaluations to start the search. Another advantage of using HEEDS is that HEEDS facilitates the process automation from CAD change to CFD calculation in Fig. 14, which significantly reduce the cost for manual operation.
5.2. Design variables and constraints

Table 2 and Fig. 15 show the design variables, objective function, and constraints set for the study of optimization. The study was aimed to improve the uniformity of vapor while maintaining the pressure drop of the current design. The number of function evaluations for the study was about 200.

Table 2 Design variables and constraints

| Design variables                  | Objective function                   | Constraint               |
|-----------------------------------|--------------------------------------|--------------------------|
| Mixer blade angle (Forward)       | Maximize uniformity index of vapor   | Pressure drop ≤ (current design) |
| Mixer blade angle (Backward)      |                                      |                          |
| Mixer position                    |                                      |                          |
| Mixer rotation angle              |                                      |                          |
| Injector boss position            |                                      |                          |
| Injector angle                    |                                      |                          |

5.3. Optimization results & correlation with visualization experiment

Figure 16 shows the search results mapped in the objective space. The results indicate that the uniformity of vapor and pressure drop are in a tradeoff relationship. As the uniformity of vapor increases, the pressure drop increases. Table 3 is a comparison between the current design and the best design found by HEEDS. A significant improvement in the vapor uniformity by 1.0 percent was achieved even while the pressure drop is also improved by 0.3 percent and the flow uniformity is kept same with current design. Those improvements were achieved by changing the mixer rotation angle of +1.5°, injector position of +2 mm, and injection angle +2.5°.

Table 3 Comparison between current design and best design

| Vapor uniformity | Flow uniformity | Pressure drop [Pa] |
|------------------|-----------------|--------------------|
| Current design   | 0.91            | 0.97               | 104.1              |
| Best design      | 0.92 (1.0% up)  | 0.97 (no change)   | 103.7 (0.3% down)  |

To get further insights into the design space, Matsumura (12) suggested identifying what limits the boundaries of objective space so that the designer can take appropriate actions to make the design even better. Figure 17 shows a parallel plot created on HEEDS, with which we can easily see trends happening in high dimension space.

Fig. 14 Automated process by HEEDS

Fig. 15 Design variables for design space exploration

Fig. 16 Search results (objective space)

Fig. 17 Parallel plot
It is obvious that the objective space is not limited by the upper or lower bounds of the design variables but by the constraint on the pressure drop. Relaxing the constraint on pressure drop or changing the design concept could be an action for further improvement.

To see overall trends of the design space, the relationship between the vapor uniformity and pressure drop with respect to the blade angles (forward and backward) was analyzed by using 3D bubble plot created on HEEDS in Fig. 18 and 19. It can be seen in Fig. 18 that the blade angle (backward) are highly related to the vapor uniformity and pressure drop. On the other hand, monotonic relationship to those responses cannot observed with respect to the blade angle (forward).

For the optimized design confirmation, we again performed the test with the same condition. Figure 20 shows the comparison of the experimental results and CAE design results. The results indicated the design variables effects the vaporization improvement.

6. Summary & Future Studies

In this study, we proposed an analysis model with low temperature flow, and water injection condition. We achieved to visualize the spray flow pattern, water distribution at cross section and well correlate them with analysis model. Best design concept has been examined with a design space exploration tool and again correlated with an experimental study. Optimization study helped to find a better design in terms of vapor uniformity while maintaining the pressure drop same as the current design. By reviewing the search results with interactive visualization tools, such as parallel plot and 3D bubble plot, we got useful insights into the designs space, for example, what limits the boundary of objective space and overall trends of design space. As future studies, we are planning to extend the study by actual engine and systems using DEF.

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References

(1) Nohara, T., " Possibilities and Utilization of Urea as the Energy Carrier," Journal of the Japan Institute of Energy, Vol.93, pp.393-401 (2014).
(2) Zheng, G., Palmer, G., Salanta, G., and Kotrba, A., "Mixer Development for Urea SCR Applications," SAE Technical Paper 2009-01-2879 (2009).
(3) Heinrich Gillet GmbH (Tenneco): Method for mixing an exhaust gas flow, U.S. Patent No. US8272777 B2 (2009).
(4) StarCCM+, Users guide, CD-Adapco (2017).
(5) Gosman, A.D., et al., “Aspects of computer simulation of liquid-fueled combustors”, AIAA, J. Energy, Vol.7, No.6, pp.482–490 (1983).
(6) Schmidt, D.P., et al., “Pressure-Swirl Atomization in the Near Field”, SAE Technical Paper Series, 1999-01-0496 (1999).
(7) Reitz, R.D., and Diwakar, R. "Effect of Drop Breakup on Fuel Sprays", SAE Technical Paper 860469 (1986).
(8) Spalding, D.B. “A standard formulation of the steady convective mass transfer problem”, Int. J. Heat Mass Transfer, Vol.1, pp.192-207 (1960).
(9) Suzuki, D., Kodama, S., Ochiai, M., Sunami, Y., and Hashimoto, H. “Visualization experiment of gas flow in dry gas seals,” Journal of Advanced Science, Vol.28(11005) (2016).
(10) Koc, S., Kim, H. J., and Nakahashi, K. “Aerodynamic Design of Complex Configurations with Junctions,” Journal of Aircraft, Vol.43, No.6, pp.1838-1844 (2006).
(11) “SHERPA - An Efficient and Robust Optimization/Search Algorithm”, www.redcedartech.com/pdfs/SHERPA.pdf, (Accessed 2013-09-04).
(12) Taiki Matsumura, “Review after optimization study: what we can learn on the boundary of objective space,” Poster session presented at The Society of Instrument and Control Engineers 2015 Conference, Hokkaido (2015).