



# The Research on Urea Nozzle Optimization of Marine Selective Catalyst Reduction (SCR) System to Reduce NO<sub>x</sub> from Marine Diesel Engines

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## ABSTRACT

Selective Catalyst Reduction (SCR) is currently the most practical method for NO<sub>x</sub> reduction of marine diesel engines. The effective use of urea depends very much upon the configuration and structure of the nozzle. This paper simulated the operation of the urea nozzle of the marine SCR system in ANSYS fluent, and utilized the Euler-Lagrange discrete phase model to calculate the droplet movement of different injection models. The simulation results show that the droplet hardly impinged on the exhaust pipe wall and the Sauter Mean Diameter (SMD) of the urea solution droplet uniformity is the best when the injection angle is at 120°.

## INTRODUCTION

Compared with other transportation methods, shipping has obvious advantages in terms of cost and productivity. Currently about 90% of international trade in mass is transported by ships. While ships are also regarded as an important source of air pollution, especially for the NO<sub>x</sub>. It is regulated by international convention that the marine diesel engines of more than 130KW output have to reduce the NO<sub>x</sub> emission to about 80% compared with the standard of 2010 in the Emission Control Area (ECA) since January 1, 2016, which is a big change in the shipping industry and gives a great pressure to the researchers on the development of NO<sub>x</sub> emission control facilities. In many alternatives of NO<sub>x</sub> reduction methods, Selected Catalyst Reduction (SCR) is regarded as the most practical and feasible one, for it has been used on land trucks for many years (Friedrich 2007). In the SCR system, reducing agent urea is injected into the exhaust pipe of the diesel engine, which will generate NH<sub>3</sub> and react with NO and NO<sub>2</sub> under the assistance of catalyst, the result is harmless N<sub>2</sub> and H<sub>2</sub>O. It is a perfect process for the NO<sub>x</sub> emission control, except the expenditure of urea which is a remarkable cost for ship operation. In this connection, the optimization of SCR system to reduce the urea consumption is very valuable.

The urea injection system controls the injection pressure, volume and timing of the urea. The nozzle plays a vital role in the injection module. Its structure and shape can affect the fine atomization of the urea solution. In order to mix the urea solution uniformly with the exhaust gas, ideally the

nozzle should be placed at the axial centre of the exhaust pipe. However, in the reality, it is difficult to fix the nozzle in the inside of the exhaust pipe. Practically, the nozzle is fixed to the wall of the exhaust pipe, for it will be more convenient for maintenance. If the nozzle sprays in an improper direction, it will cause the deposition of urea and pipe corrosion. Therefore, it should be installed at an angle with the axis of exhaust pipe, this angle is called injection angle. The injection angle is closely linked with the penetration distance, cone angle of the spraying and the mixing degree of urea and exhaust gas. In this paper, the injection angle will be simulated and analysed in order to find out the best structure and configuration of urea nozzle.

## THE MATHEMATICAL MODEL

The injection of urea solution will atomize the solution into tiny droplets. The droplet can be regarded as discrete phase, while the exhaust gas is a continuous phase. Therefore, we can calculate this process based on the Euler-Lagrange discrete phase model. For turbulence, the  $k-\epsilon$  model can be used (Ding 2003).

**Mathematical model of continuous phase:** Fluid flow is mainly controlled by the law of conservation of the physical, for example, the mass conservation equation, momentum conservation equation, energy conservation equation and so on (Ding 2003). No matter what the kind of flow or liquid, it must comply with the three equations.

Mass conservation equation is also called the continuous phase equation. The law of conservation of the quality

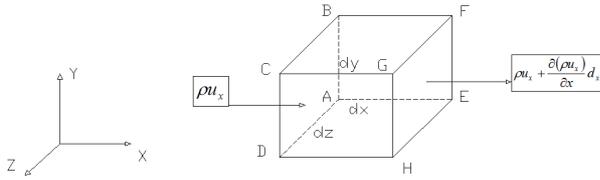


Fig. 1: The law of conservation of the quality of the schematic diagram for the X axis direction.

of the schematic diagram for the X axis direction is shown in Fig. 1.

Continuity equation under the differential form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad \dots(1)$$

Continuity equation is applicable to any situation, whether for viscous, compressible and stationary flow. For stationary flow and unsteady flow, expression of mass conservation equation is different.

Momentum conservation equation is divided into the viscous momentum conservation equation and non-viscous momentum conservation equation.

Navier-stokes equations (Ding 2003):

$$\rho \frac{du}{dt} = \rho * F_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) + \frac{\partial}{\partial x} \left[ \frac{\mu}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \quad \dots(2)$$

$$\rho \frac{dv}{dt} = \rho * F_y - \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial v}{\partial z} \right) + \frac{\partial}{\partial y} \left[ \frac{\mu}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \quad \dots(3)$$

$$\rho \frac{dw}{dt} = \rho * F_z - \frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left( \mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial w}{\partial z} \right) + \frac{\partial}{\partial z} \left[ \frac{\mu}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \quad \dots(4)$$

Navier-stokes equation can more accurately describe the actual flow, but the Navier-stokes equation has nonlinear term. Compared with the numerical solution, the general analytic solution is difficult to get by the Navier-Stokes equation, except the boundary conditions are easy to be calculated.

Energy conservation equation is expressed as the exchange rate of the momentum and internal energy within the volume,  $\tau$  is equal to the power of mass force and surface force per unit time plus heat absorbed within the volume per unit time.

Energy conservation equation:

$$\rho c \frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda \frac{\partial t}{\partial y} \right) + \frac{\partial}{\partial z} \left( \lambda \frac{\partial t}{\partial z} \right) + \phi \quad \dots(5)$$

In this equation,  $t, \rho, \phi, c$  and  $\lambda$  represent the

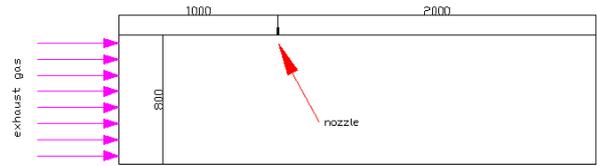


Fig. 2: The position of the nozzle in the exhaust pipe.

temperature, fluid density, heat generated per unit time and volume, specific heat capacity and thermal conductivity respectively.

**Mathematical model of discrete phase:** The simulation of discrete phase in the FLUENT software is conducted under the Lagrangian coordinates. The track equations of particles in discrete phase are established by the differential equation of forces on the particles (Huang 2011). The particle inertia force is equal to total force on the particles. The force balance equation in the cartesian coordinates on the X direction is:

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad \dots(6)$$

In this equation,  $F_D(u - u_p)$  represents the drag force per unit mass of particle, in which,

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D R_e}{24} \quad \dots(7)$$

with

$$R_e = \frac{\rho d_p |u_p - u|}{\mu} \quad \dots(8)$$

In which,  $u, u_p, g_x, \rho_p, d_p$  and  $R_e$  represent velocity of fluid, particle velocity, particle dynamic viscosity, particle density, particle diameter and relative particle Reynolds number, respectively.

Mild microscopic particles are particles with the diameter of 1-10 microns. Stokes drag force equation is applicable to the mild microscopic particles.

$F_D$  is defined as:

$$F_D = \frac{18\mu}{d_p^2 \rho_p C_c} \quad \dots(9)$$

with

$$C_c = 1 + \frac{2\lambda}{d_p} (1.257 + 0.4e^{-(1.1d_p/2\lambda)}) \quad \dots(10)$$

In this equation,  $C_c$  represents the Cunningham correla-

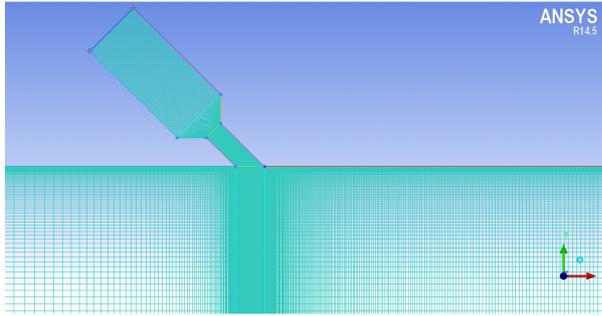


Fig. 3: Local figure of nozzle meshing.

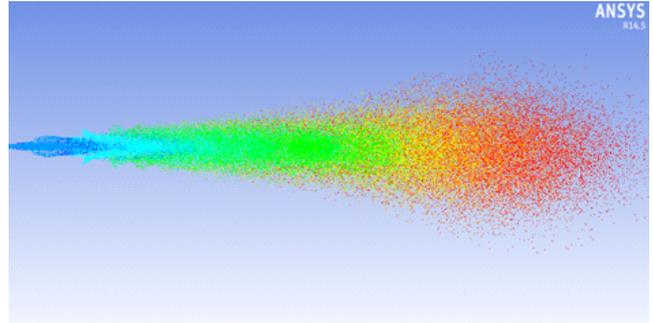


Fig. 5: Spray field of numerical simulation.

tion (Huang 2011) of Stokes drag equation, taking into account the rectified gas mechanics correlation in particle wall velocity slip.

Particle track equation:

$$\frac{d_x}{d_t} = u_p \quad \dots(11)$$

Particle track equation calculate the particle in the process of fluid motion trajectory equation. The equation is based on time step and calculated through step-by-step integration. The equations can also add particle mass equation and heat transport equation, by which the velocity, mass, temperature of every particle can be acquired.

**ESTABLISHMENT AND VERIFICATION OF THE NOZZLE MODEL**

**The calculation model:** To study the effect of wall impingement of marine urea injection, optimizing the location of nozzle and take into account the actual situation of diesel engine, the study assumed that the diameter of the exhaust pipe is 800mm, the axial distance from inlet of exhaust to nozzle is 1000mm, and axial distance from nozzle to outlet is 2000mm.

After the nozzle geometric model was set up, the structure grid of nozzle should be used. Because of the complexity of flow situation, it is necessary to increase the density around the nozzle for more accurate solutions. Fig. 3 shows the quality of nozzle meshing reached 0.9, which is satisfied with requirements.

The study utilizes the coupling calculation method so that the energy equation should be turned on and turbulence

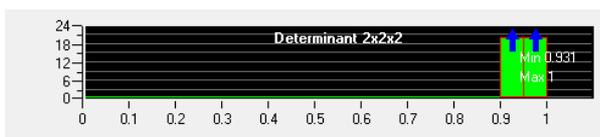


Fig. 4: The quality of meshing.

flow equation should be used to calculate continuous phase flow field. Turbulence model using the RNG  $k-\epsilon$  model because the gas phase flow is highly turbulent. Since the coupling is calculated between liquid and gas, component transport model is needed. Mixture includes urea solution as discrete phase and exhaust gas as continuous phase. After continuous phase calculation converged, the discrete phase model was introduced in the computational domain in order to calculate the track of discrete phase droplets.

This study has two kinds of material: urea solution and exhaust gas. Urea solution is urea aqueous solution containing 32.5% urea. Table 1 gives the physical parameter of urea solution under 300K and 1 bar (Strom et al. 2009). Exhaust gas can be regarded as compressible ideal gas whose parameter is default in Fluent.

**Verification of calculation model:** Fig. 5 shows distribution map of the numerical simulation of particles changed with time. From this picture, the particles distributed as conical on the whole. The particles at the outer part of the particle beam are smaller and the inner ones are larger. Along the direction of injection, the further the distance, the smaller

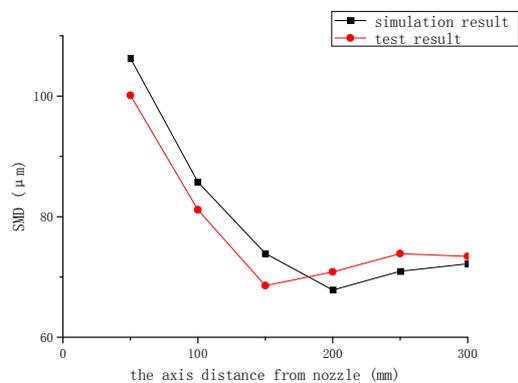


Fig. 6: The droplet SMD value distribution where the axis distance from the nozzle.

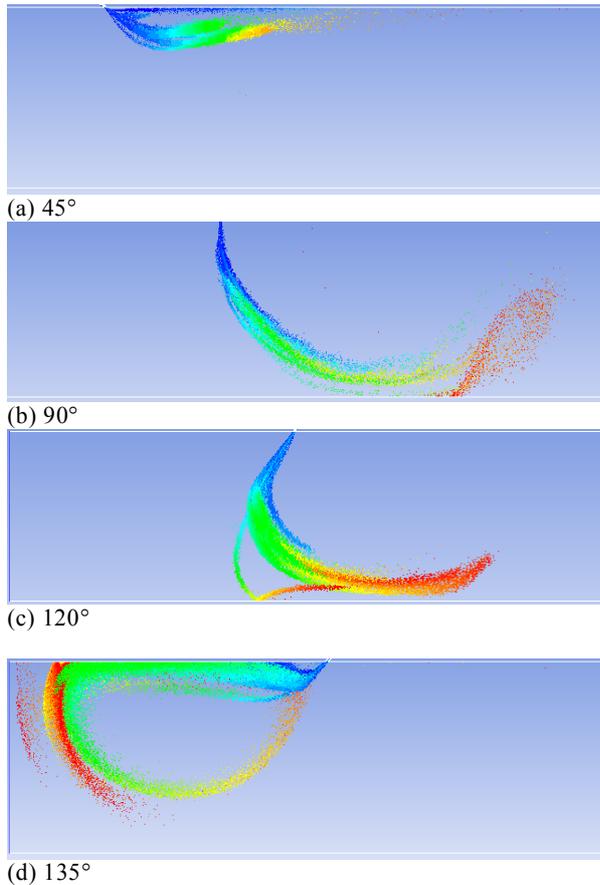


Fig. 7: Four different morphology of injection.

the particle diameter, and the particle size distribution became more and more dispersed, which conformed to the actual situation.

This study uses the Sauter Mean Diameter (SMD) to represent the particle size. SMD translates the particles into a sphere with constant surface area and volume, the diameter of the sphere is SMD. This study carried out the numerical simulation under the same working condition as the study carried by Li et al. (2006) which is a real experiment carried out. Fig. 6 shows that the simulation result is trustable.

### EFFECTS OF WALL IMPINGEMENT AT DIFFERENT INJECTION DIRECTION OF UREA

**The morphology of injection:** This study carried out CFD simulation in four different injection direction (45°, 90°, 120°, 135°) with injection pressure 2.5MPa (gauge pressure), the velocity of exhaust gas 30m/s and mass flow of urea solution 60g/s. The injection morphology of four different directions is shown in Fig. 7

At the injection direction of 45°, some droplets blew to the wall of exhaust pipe, and evaporated due to high tem-

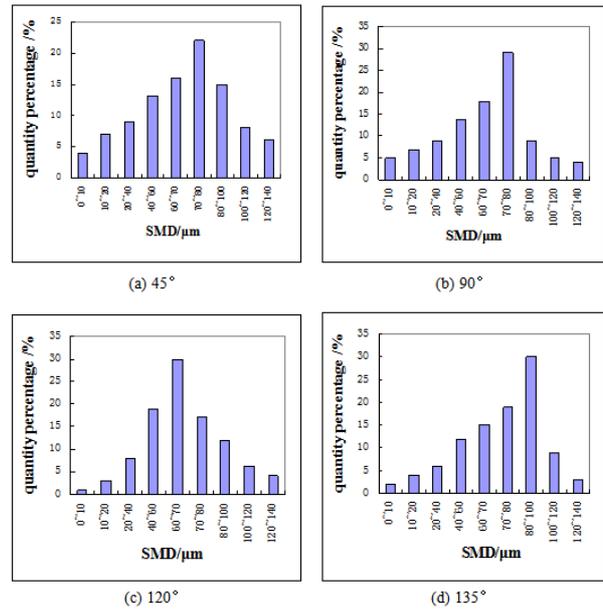


Fig. 8: Probability distribution of the SMD value.

perature, which resulted in considerable reduction in the number of droplets, and worse, mixing effect of droplets and exhaust gas.

At the injection direction of 90°, the droplets were blown to the upper pipe wall, but a small number of them were injected to under pipe wall and rebounded because of collision. At the injection direction of 120°, droplets had no collision with the exhaust pipe basically and had a good mixture with exhaust gas.

At the injection direction of 135°, due to the reversal injection angle being too steep, some droplets blew to the pipe wall directly under the injection velocity and gas velocity, which resulted in energy loss of a large number of droplets to form a small amount of crystallization. After the droplets collided to the pipe wall, vortices which enhanced the mixture of droplets and exhaust gas would have been generated by the gas flow in local areas.

Four cases of droplet diameter distribution are shown in Fig. 8. At the injection direction of 45°, the value of SMD mainly distributed in the range of 60 to 80. As the injection angle increased, the value of SMD decreased gradually. At the injection direction of 120°, the value of SMD mainly distributed in the range 40 to 60. If the injection angle continues to increase, the value of SMD would increase as well. The reason is that the droplets were affected by the carrying action and crushing action of the exhaust gas. The carrying action is that the exhaust gas carry droplets to backward position of the pipe and as a result the diameter of droplets increases. The crushing action is that the droplets were de-

Table 1: The physical parameters of urea solution.

Physical parameter	Reference
Density (kg/m <sup>3</sup> )	1330
Specific heat (J/kg-k)	4177
Thermal conductivity (W/m-k)	0.0454
Viscosity (kg/m-s)	0.0016
Vapor pressure (MPa)	0.6
Heat of vaporization (J/kg)	3,095,995
Surface tension (N/m)	0.0777

Table 2: The results of CFD simulation for four different injection angle.

Angles/diameter	45°	90°	120°	135°
$d_{0.1}$ (μm)	18.12	17.16	36.79	35.72
$d_{0.5}$ (μm)	71.34	67.90	63.15	71.34
$d_{0.9}$ (μm)	110.49	101.31	100.27	129.01
$s$	1.294	1.239	1.005	1.308

composed into smaller diameter droplets as a result of the kinetic energy of gas.

At the injection direction of 45°, the droplets were greatly influenced by the carrying action than the crushing action, so that the ones with large diameter were moved from upstream to downstream with the exhaust gas, which resulted in the increase of number of large diameter ones. At the injection direction of 90°, the crushing action play more important role. The large droplets decomposed into small droplets, which resulted in the increase of large droplets and decrease of small droplets. With the injection angle increasing, the injection of axis direction intersected with the exhaust gas motion direction which is called reversal injection. The relative velocity of droplets and exhaust is very large so that the droplets collided with the gas flow and broke violently. Also, the reversal injection increased the stay time for urea solution in the exhaust pipe, which is a benefit to the urea decomposition of atomization.

At the injection direction of 120°, the value of SMD was the smallest. With the angle increased, some droplets decomposed and were blown to the pipe by exhaust gas because of the narrow space. At the injection direction of 135°, the SMD distribution of droplets shows that the diameter of droplets increased.

**Uniformity:** The uniformity of distribution is important for the urea solution to mix with nitrogen oxides in the exhaust and catalyst reaction efficiency. But most of the researches only studied qualitative analysis by the picture of spray filed, which could not accurately and quantitatively reflected the uniformity of droplets (Liu et al. 2008). This study defined the uniformity by probability statistics and

quantitative analysis.

Based on the related literatures and combined with the knowledge of mathematical statistics (Li et al. 2006), this paper use the formula in equation 12, to define the uniformity. The diameter distribution of the droplets is measured by droplets dispersion.

$$S = \frac{d_{0.9} - d_{0.1}}{d_{0.5}} \quad \dots(12)$$

Where, S represents the droplets dispersion,  $d_{0.1}, d_{0.5}, d_{0.9}$  represents the droplets of three different diameters. Mass percentage of droplets that the diameter less than  $d_{0.1}, d_{0.5}, d_{0.9}$  represented 10%, 50%, 90%, respectively. Here the smaller S value means that the diameter distribution of droplets is more concentrated, uniform atomization, small dispersion and good quality of atomization.

The results of uniformity calculation for 45°, 90°, 120°, 135° injection, demonstrated that the droplets of uniformity decreased when the injection angle increased. At the injection angle of 120°, the uniformity is the best. If the angle is continued to add, the droplets uniformity will worsen. Table 2 shows the results of the CFD simulation.

From the Table 2, we can summarize that the injection angle has great influence on the diameter distribution uniformity of the droplet. At the injection direction of 45°, some droplets injected into the pipe and some droplets adhered to pipe wall and slid along the wall pipe. During the sliding, the atomized droplets get together and become larger, so that the proportion of large diameter droplets will be higher, and the proportion of small diameter droplets lower. At the injection direction of 90°, the radial velocity was the maximum and the axis velocity was the minimum. Droplets on the distribution of the exhaust pipe bottom increased and the number of droplets decreased along the Y positive axis. Compared with the 45°, more droplets were broken by exhaust gas. The droplets uniformity become better because of the intensive air force and droplets evaporation. At the injection direction of 120°, the injection is so called reversal injection. After the urea solution was inject into the pipe, the larger diameter droplets were broken into small droplets by more intensive air force due to the higher relative velocity between droplets and exhaust gas. During the process, the tiny droplets would gather together again to decrease the much fine droplets. Compared with the 90°, the radial velocity of 120° is lower. Droplets will not concentrate in the lower part of the exhaust pipe and the space distribution is more uniform. At the injection direction of 135°, the droplets uniformity become worsen. The reason is that, most of the droplets were blown to the pipe wall and a large number of droplets adhered to pipe wall to form the crystal,

because the injection angle was too steep and the velocity was too fast.

## CONCLUSION

The aim of the presented work is to study the wall impingement of the urea nozzle of marine SCR system through CFD-simulations based on a mathematical model of continuous phase and discrete phase. The method is verified by the experiment results. Therefore the simulation results were accurate and reliable.

Four different injection angles ( $45^\circ$ ,  $90^\circ$ ,  $120^\circ$ ,  $135^\circ$ ) were simulated. Through intuitive performance of atomization morphology and quantitative simulation results, droplets have no collision with exhaust pipe and have a good mixture with exhaust gas when the injection angle is  $120^\circ$ .

It is also proved that the uniformity of diameter distribution is the best at this angle.

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