

# Simulation and Optimization of SK Mixer in SCR System of a Diesel Engine

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## Abstract

According to the operation parameters of a diesel engine SCR system, a three-dimensional numerical model of SK mixer in SCR system is established by calculating the component transport and chemical reaction model and discrete phase model of (CFD). The influence of SK mixer on SCR system is analyzed from two aspects of reducer uniformity index and pressure loss. Through the orthogonal test, the length-diameter ratio, torsion angle and downstream distance from the nozzle of SK mixer are analyzed, and the best optimization scheme is obtained. It is found that the SK mixer can cause strong swirl and turbulence of the reducing agent, which can greatly improve the uniformity of ammonia distribution, and when the SK mixer with a length-diameter ratio of 1.2 and a torsion angle of  $180^\circ$  is twice the diameter of the exhaust pipe downstream of the nozzle, the effect of ammonia mixing is the best.

## Keywords

SCR System; CFD; SK Mixer; Orthogonal Test.

## 1. Introduction

SCR technology, also known as selective catalytic reduction technology, originated in the United States, and then improved by Japan, it was applied to the NO<sub>x</sub> control of thermal power plant boilers. In order to meet the NO<sub>x</sub> control standards of IMO Tier I, Tier II and Tier III, SCR technology has been widely used in tail gas denitrification of large merchant ships in the past two decades because of its excellent denitrification ability and good economy.

The denitrification ability of SCR system is closely related to the flow field distribution of reductant. If the local reductant is excessive or insufficient, it will lead to the decrease of denitrification rate and the increase of ammonia leakage.

Therefore, in order to improve the uniformity of the reducing agent flow field, one or two static mixers are generally set up downstream of the nozzle, which causes a strong swirl when the reducing agent follows the tail gas flow through the mixer and avoids local instability.

Static mixer is a kind of fluid mixing device without moving parts. Compared with dynamic mixer, it has the advantages of simple structure, easy maintenance, good stability and good economy, so it is very suitable to be used in marine SCR system.

In the application of industrial engineering, there are many kinds of static mixer. At present, there are mainly eight standard static mixer types in China: SK, SV, SZ, SL, SY, SD, SH, SX.

Among them, SK static mixer has spiral blade shape, good mixing performance and simple structure, so it is suitable to be used as static mixer in SCR system.

In this paper, the SCR system of a marine diesel engine is taken as the research object. Through computational fluid dynamics (CFD), orthogonal tests are carried out on three levels of length-diameter ratio, torsion angle and downstream distance from the nozzle of SK mixer, and the best mixing scheme is obtained.

## 2. Numerical model of SCR system

### 2.1 SCR system

The SCR system is mainly divided into four parts: the mixing part, the expansion tube, the main body of the reactor and the shrinkage tube.

The main size of the SCR system reactor of marine diesel engine studied in this paper is the cylindrical shape of 1800mmx1432mm, the expansion angle is 70 degrees, and the diameter of exhaust pipe D is 660mm. See Fig. 1.

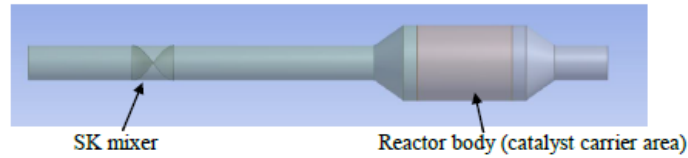


Fig. 1 Schematic diagram of SCR system

The focus of this paper is on the mixing part of the SCR system, that is, the inlet section of the nozzle-mixer-expansion tube, as shown in Fig. 2:

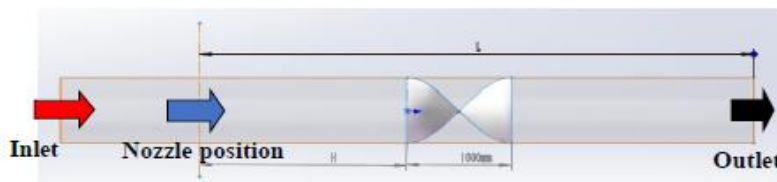


Fig. 2 Geometric model of mixer

Note: H is the distance from the front end of the mixer to the nozzle, and L is the distance from the nozzle to the outlet (expansion tube inlet).

**2.2 Nozzle parameter setting**

Nozzle arrangement parameters, see Table 1.

Table 1. Nozzle layout parameter table

Nozzle parameters	Type	Number	Arrangement mode	Inner diameter	Distance from nozzle to outlet
Scheme	Air-blast- atomizer	6	Circumferential arrangement at 4 /D	0.5mm	8D

Note: D is the diameter of exhaust pipe.

**2.3 SK static mixer model**

The SK static mixer is made of a cuboid steel plate screw at a certain angle, see Fig. 3, and is close to the exhaust pipe wall with a thickness of 1mm, which is only 660 of the exhaust pipe diameter D=660mm, so in numerical modeling, in order to reduce the number of grids and some unnecessary computing resources, the mixer can be regarded as a thin sheet and its thickness can be ignored.

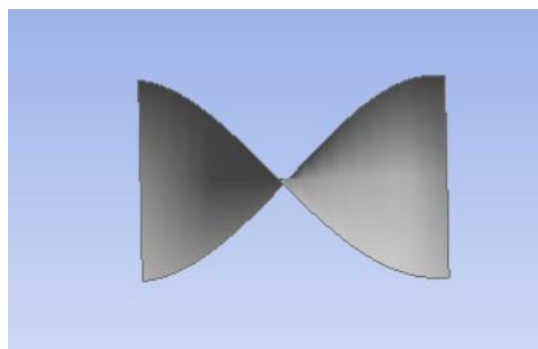


Fig. 3 Geometry model of SK mixer

## 2.4 Meshing and boundary conditions

### 2.4.1 Meshing

The simulation model mesh used in this paper is a mixed grid of tetrahedron and hexahedron, and a boundary layer is added to the pipe wall and the boundary of the mixer, see Fig. 4.

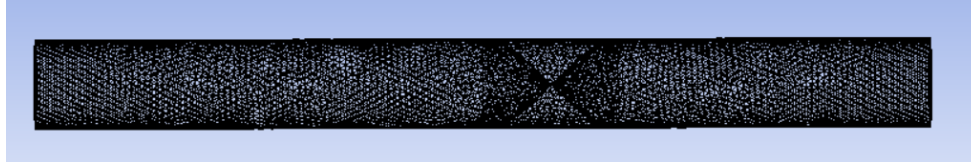


Fig. 4 Schematic diagram of meshing

### 2.4.2 Boundary conditions

The boundary conditions of the numerical simulation in this paper are shown in Table 2.

Table 2. Boundary condition table

Inlet(velocity)	velocity	Temperature	Hydraulic diameter	Turbulence intensity
	20m/s	400°C	660mm	5%
Outlet(pressure)	/	Temperature	Hydraulic diameter	Turbulence intensity
	/	400°C	660mm	5%
Wall	No slip	viscous flow	heat insulation	/

## 3. Numerical model

The physical and chemical reactions of the mixed part of SCR system are mainly spray atomization of urea aqueous solution and evaporation hydrolysis process. The numerical models of the process include continuity equation, momentum conservation equation and energy conservation equation, and the turbulence model chooses RNG. K-epsilon model, component transport and chemical reaction model choose eddy dissipation conceptual model (EDC); nozzle atomization simulation chooses discrete droplet model (DDM).

### 3.1 Continuity equation

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \bar{u}) = 0 \quad (1)$$

Note:  $\rho$  is the density;  $t$  is the time;  $\bar{u}$  is the velocity vector along the direction of  $x$  and  $y$ .

### 3.2 Momentum conservation equation

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u u)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} + \frac{\partial(\rho u w)}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( u \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( u \frac{\partial u}{\partial z} \right) - \frac{\partial p}{\partial x} + s_u \quad (2)$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho v u)}{\partial x} + \frac{\partial(\rho v v)}{\partial y} + \frac{\partial(\rho v w)}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( u \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left( u \frac{\partial v}{\partial z} \right) - \frac{\partial p}{\partial y} + s_v \quad (3)$$

$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho w u)}{\partial x} + \frac{\partial(\rho w v)}{\partial y} + \frac{\partial(\rho w w)}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left( u \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial z} \left( u \frac{\partial w}{\partial z} \right) - \frac{\partial p}{\partial z} + s_w \quad (4)$$

Note:  $\mu$  is the dynamic viscosity,  $s_u$ ,  $s_v$ ,  $s_w$  are the generalized source terms of the momentum conservation equation, since the ship tail gas is assumed to be incompressible flow, it is advisable to take  $s_u$ ,  $s_v$ ,  $s_w$  as 0.

### 3.3 Energy conservation equation

$$\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho u T)}{\partial x} + \frac{\partial(\rho v T)}{\partial y} + \frac{\partial(\rho w T)}{\partial z} = \frac{\partial}{\partial x} \left( \frac{k}{C_p} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{k}{C_p} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{k}{C_p} \frac{\partial T}{\partial z} \right) + s_T \quad (5)$$

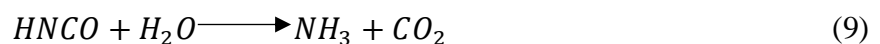
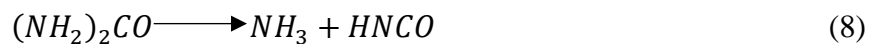
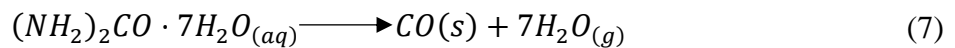
Note:  $T$  is the temperature;  $C_p$  is the specific heat capacity;  $k$  is the heat transfer coefficient of the fluid;  $s_T$  is the viscous dissipation term of the fluid.

### 3.4 Component transport equation

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (6)$$

Note:  $Y_i$  is the mass fraction of a component,  $\rho$  is density,  $\vec{J}_i$  is the diffusion of substances in I,  $R_i$  is the net production rate of chemical reaction,  $S_i$  is the additional production rate.

The chemical reactions involved in this paper should be:



## 4. Evaluation Standard of flow Field in mixed part of SCR system

### 4.1 Ammonia concentration uniformity index

The evaporation, hydrolysis and injection of urea aqueous solution is a very complex chemical reaction process. In order to study the effect of different parameters on the uniformity of ammonia concentration, it is necessary to give a reasonable evaluation index.

Therefore, in this paper, the uniformity index is introduced to quantitatively analyze the change law of urea aqueous solution in the reaction process.

Uniformity index is a commonly used evaluation index in the study of gas flow and distribution.

In this paper, the uniformity index based on component distribution is mainly used to monitor the ammonia concentration distribution in the front section of the catalyst inlet.

Uniformity index based on concentration distribution:

$$\gamma = 1 - \frac{1}{2n} \sum_{i=1}^n \frac{\sqrt{(C_i - \bar{C})^2}}{\bar{C}} \quad (10)$$

Note:  $\gamma$  is the uniformity index,  $0 < \gamma < 1$ ,  $n$  is the number of grids on the monitoring section,  $C_i$  is the parameter value on the grid I, and  $\bar{C}$  is the average value of the parameters on the whole cross section.

The cross section monitored in this paper is the inlet end of the expansion tube (catalyst inlet section). The more uneven the ammonia concentration distribution on the cross section is, the smaller the uniformity index  $\gamma$  is, and the lower the denitrification rate of SCR system is. On the contrary, the more uniform the ammonia concentration distribution is, the higher the uniformity index  $\gamma$  value is, and the higher the denitrification rate of SCR system is.

### 4.2 Pressure loss

The pressure loss is the pressure difference between the inlet and the outlet. Excessive pressure loss will lead to an increase in diesel engine fuel consumption.

Pressure loss (Pa):

$$\Delta P = P_{in} - P_{out} \quad (11)$$

Note:  $P_{in}$  is the inlet pressure;  $P_{out}$  is the outlet pressure

## 5. Orthogonal Experimental Design of SK static Mixer

Orthogonal experimental design is a common scientific experimental method, which is mostly used in multi-factor and multi-level experimental design.

The orthogonal experimental design is to select some representative points with "uniform dispersion and neat comparability" on the basis of the comprehensive experimental design. compared with the comprehensive test, it greatly shortens the number of experiments and is a highly efficient experimental design method.

In this paper, the length-diameter ratio  $K$ , torsion angle  $C$  and spray distance  $H$  of SK static mixer are selected as the three factors affecting the uniformity of flow field, and three levels are selected from each of the three factors, as shown in Table 3.

Table 3. Orthogonal test factors and level table

Number	K	C	H
1	1.2	90°	1D
2	1.5	120°	1.5D
3	2.0	180°	2D

### 5.1 Orthogonal test table

Taking the ammonia concentration uniformity index  $\gamma$  and pressure loss  $\Delta P$  at the outlet as the final evaluation index, according to the orthogonal test scheme of three factors and three levels, the orthogonal table of  $L_9(3^4)$  was selected for orthogonal test.

The method of numerical simulation test is adopted in this paper. in order to reduce the test error in calculation, each group of data is calculated three times to take the average value.

The specific schemes and results are shown in Table 4:

Table 4. Orthogonal test table

Number	K	C	H	$\gamma$	$\Delta P$
1	1.2	120	D	0.9034	37.10
2	1.2	150	2D	0.9196	55.20
3	1.2	180	1.5D	0.9635	75.47
4	1.5	120	1.5D	0.8763	27.33
5	1.5	150	D	0.8941	37.97
6	1.5	180	2D	0.9409	55.20
7	2.0	120	2D	0.8355	18.97
8	2.0	150	1.5D	0.8587	24.93
9	2.0	180	D	0.9040	33.69

### 5.2 Analysis of the results of orthogonal test.

The common methods for analyzing the results of orthogonal experiments are range analysis and variance analysis.

#### 5.2.1 Range analysis

The range analysis method is to evaluate the influence effect of each single factor by comparing the range  $R$  of the response value at different levels of a single factor. this analysis method is more intuitive and can quickly find the primary and secondary factors in the experiment, also known as the intuitive method.

In this experiment, the influence degree of each single factor is analyzed according to the ammonia concentration uniformity index and the range of pressure loss, and the optimal collocation scheme is selected according to different indexes.

A) The table below is the response table of ammonia concentration uniformity index.

Table 5. Ammonia concentration uniformity index response table

	K	C	H
1	0.9387	0.8742	0.9327
2	0.9132	0.8877	0.9262
3	0.8759	0.9107	0.9234
Range value	0.0628	0.0365	0.0093
Best scheme	1	3	1

According to the analysis of the data in the table 5, the effects of length-diameter ratio, torsion angle and spray distance on ammonia concentration uniformity index are as follows:  $K > C > H$

If only the realization of the maximum ammonia concentration uniformity index is considered, the optimal scheme of SK static mixer is:  $K=1.2$   $C=180^\circ$   $H=1D$ . Write it down as:  $K1C3H1$

B) The following table is the pressure loss response table

Table 6. Pressure loss response table

	K	C	H
1	73.86	27.19	51.58
2	52.90	38.10	51.75
3	33.87	52.92	52.18
Range value	39.99	25.73	0.6
Best scheme	3	1	1

According to the analysis of the data in table 6, the effects of aspect ratio, torsion angle and spray distance on pressure loss are as follows:  $H < C < K$

If only the minimum pressure loss is considered, the optimal scheme of SK static mixer is:  $K=2.0$   $C=120$   $H=1D$ . Write it down as:  $K3C1H1$

### 5.2.2 Variance analysis method

Analysis of variance is often used to determine whether multiple control variables have a significant impact on the test results, and the analysis of variance can also determine whether the test results are caused by test errors.

In this paper, repeated experiments have been used to reduce the test error, so in the following analysis of variance, only the influence of various factors on the test results is considered.

After the data of orthogonal table were processed by SPSS software, the ANOVA table of ammonia concentration uniformity index and the ANOVA table of pressure loss were obtained.

A) Variance analysis of ammonia concentration uniformity index

Table 7. Analysis of variance table of ammonia concentration uniformity index

	Class III sum of squares	Degree of freedom	Mean square	F	Significance
K	0.006	2	0.003	350.341	0.0285
C	0.007	2	0.003	384.077	0.0260
H	5.056e-06	2	2.528e-06	0.296	0.7718

From the significance of the Table 7, we can see that the torsion angle  $C < \text{length-diameter ratio } K < 0.05 < 0.1 < \text{spray distance } H$ , so the torsion angle and length-diameter ratio have significant influence on ammonia concentration uniformity index. and the influence of torsion angle is slightly greater than the aspect ratio, while the spray distance has little effect on the uniformity index of ammonia concentration.

B) Pressure loss variance analysis table

Table 8. Pressure loss variance analysis table

	Class III sum of squares	Degree of freedom	Mean square	F	Significance
K	1361.185	2	680.593	20.646	0.046
C	1019.187	2	509.594	15.459	0.061
H	74.937	2	37.469	1.137	0.468

From the significance of the Table 8, it can be seen that the length-diameter ratio  $K < 0.05 < \text{torsion angle } C < 0.1 < \text{spray distance } H$ , so the length-diameter ratio K has a significant effect on the pressure



loss, and the torsion angle C has a certain influence on the pressure loss. The effect of spray distance H on pressure loss is small.

### 5.3 Determination of the best scheme

Through the range analysis and variance analysis of orthogonal experimental design, the influence of torsion angle and aspect ratio should be given priority to when choosing the best scheme, and then the influence of spray distance should be taken into account. Small pressure loss can be achieved under the condition of ensuring the uniformity of the maximum ammonia concentration.

For the uniformity index of ammonia concentration of K, level1 > level2, the difference of pressure loss between them is in 21Pa, and the pressure drop for the whole SCR system is within an acceptable range, so the K is chosen to be 1.2.

For the ammonia concentration uniformity index of C, level 3 > level 2, the difference of pressure loss between them is less than 11pa, which is within the acceptable range, so the C is 180°

For the H, the uniformity index of ammonia concentration is the highest and the pressure loss is the smallest at level 1, so the H is D.

## 6. Conclusion

According to the analysis of orthogonal test, the ratio of length to diameter and torsion angle of SK mixer have great influence on the mixing degree of reducer. If only the single factor variable is considered and within the range of factors in this paper: (1) with the increase of torsion angle, the reductant concentration uniformity index at the entrance of the expansion tube increases gradually, but the strong swirl will also increase the pressure loss. (2) with the increase of the aspect ratio, the reductant concentration uniformity index and pressure loss at the entrance of the expansion tube decrease gradually, (3) with the increase of spray distance, the reductant uniformity index decreases slightly, and the pressure loss has no obvious change.

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