

Multiphase Modelling of SCR Systems: Using the Taguchi Method for Mixer Optimisation

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ABSTRACT

Selective catalytic reduction (SCR) systems have become the preferred technology to deal with NO_x emissions in Diesel engines. Their efficiency is highly reliant, among other factors, on the uniformity of distribution - known as Uniformity Index (UI) - of NH₃ which is injected into the system through a urea-water solution (UWS). SCR system make use of a mixer component designed to achieve the desired UI levels. However, the great variety of exhaust systems, makes it impossible to employ a universal solution. Therefore, each SCR system requires of a tailor made mixer, capable of achieving the required UI, while preventing urea crystallisation and minimising pressure drops. Computer fluid dynamics (CFD) tools together with optimisation techniques based on the design of experiments (DoE) can be used to obtain the appropriate mixer design.

This study presents a Taguchi (L4) DoE for a series of multi-phase numerical analyses, computed with the commercial software AVL Fire 2014 v, to measure the impact of three factors - the mixer blade's number (X1) and angle (X2), and the distance between the injection point and the mixer (X3) - in the performance of an SCR system, specifically NH₃ UI, Midcone pressure drop and Wall film formation. The analysis consisted of a completely mixed turbulent flow, solved using a two equations turbulence model (k- ϵ). The interaction of the injected particles was solved with an Euler/Lagrange approach, the liquid phase calculation was based on the statistical Discrete Droplet Method interacting with the numerical solution of the conservation equations of the flow pattern.

It was found that blade angle had a major impact on performance, the impact of number of blades was dependent on the blades angle, while the distance from the injector had minimum impact in performance apart from Midcone pressure drop, where a mixer closer to the injector helped to reduce pressure drops. Moreover, a linear regression model was used to predict the output of three Cases (A, B, and C), finding good agreement between the predicted results and the CFD calculated performance.

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INTRODUCTION

Over 45 years ago, automobiles began using catalytic systems for the abatement of pollutants generated by the internal combustion engine (ICE) [1]. With the passage of time, stringent environmental regulations demanded for tighter emissions control in vehicles. The particular condition of Diesel engines, which operate at lower temperatures and a larger excess of air than gasoline engines, lead to the introduction of SCR systems which make use of a reduction agent, namely ammonia NH₃, to decompose nitrogen oxides (NO_x) into nitrogen and water. Such reactions are favored in the presence of oxygen [2], a condition that fits with the operation of Diesel engines.

The tasks of an SCR system is to reduce the maximum amount of NO_x emissions without affecting the engine performance. Thus, in order to catalogue the efficiency of SCR systems it is necessary to measure performance in relation to various parameters e.g. reduction

of emissions and system pressure drop. Various studies have linked the emission reduction efficiency with the uniformity of distribution, or uniformity index (NH₃ UI) of the injected UWS, the better the distribution the higher the emissions reduction [3]. The NH₃ UI has become a popular parameter to measure the efficiency of SCR systems in CFD simulations [4].

The incomplete decomposition of the UWS can promote urea crystallisation, a common byproduct of SCR systems; Temperature appears to be one of the main factor that triggers it [5]. Urea decomposition starts at 80°C, nevertheless, complete decomposition of NH₃ occurs only above 180°C [6]. Moreover, byproducts such as cyanuric acid (C₃H₃N₃O₃), biuret (H₂N-CO-NH-CO-NH₂), melamine, ammelide, and ammeline may still form at temperatures of between 180°C and 250°C [5]. Corrosive byproducts deposition, wall wetting at the exhaust pipes, know as wall film formation,

might keep growing during the engine operation course; Leading to material damage, increased engine back pressure, and decreasing NOx reduction performance of the SCR system [7].

This study focused on improving the performance of an SCR system by improving NH₃ UI, reducing Wall film formation (urea crystallisation) and Midcone pressure drop by means of a Taguchi (L4) DoE.

Statistical design of experiments (DoE) and Taguchi optimisation techniques have been widely used and documented in automotive industry. Ganapathy et. al. (2009) used an L16 Taguchi array of experiments, considering 10 design factors at two levels, for the optimisation of a Jathropa Biodiesel engine [8]. Chen & Tan, (2012) worked on the mathematical modeling and optimisation of an SCR system using the computational software COMSOL. The optimisation technique, integrated the Taguchi method, a real-coded genetic algorithm and a neural network auxiliary model. Their study focused on the effects of three parameters including gas hourly space velocity (GHSV), operating temperatures and ammonia content on the NOx conversion (NH₃/NOx ratio); their work was based on improving NOx reduction through the optimisation and control of operation parameters (e.g. UWS injection) [9]. Seo (2011) worked on the optimisation of a EURO V SCR system for a heavy duty truck, and a Japan 2009 DPF+SCR system for an express bus. He focused on five design targets: Improvement of NOx reduction efficiency, improvement of noise reduction performance, meet exhaust back pressure requirements, minimize package volume, and minimize the urea deposit. His study presented an L18 Taguchi DoE, with 8 factors and three levels for purposes of shape and robust design optimisation, and managed to reduce urea deposits from 8g to 0g on crystallisation, and a reduction from 14.3g to 5g on urea deposit specs [5]. Arrowsmith, Bott, & Bush, (2006) used a full factorial DoE consisting of three factors at two levels (2³), and a further fractional factorial DoE at a refined experimental space to optimise the design of an SCR mixer, reporting improvements of between 2 and 26% for emission and noise reduction. They found that the mixer length, diameter and the injection spray angle (UWS) had significant effects on the removal of NOx [10].

The use of DoE techniques coupled with CFD tools can help reducing manufacturing and computational costs during the design stage of an SCR system.

METHODOLOGY

Taguchi DoE

There are well tried and document methods for the efficient design of experiments in order to gather the maximum amount of information for a particular amount of effort [11]. Taguchi DoE is an experimental technique widely used in lean methodologies such as Design for Six Sigma (DFSS) [12]. The Taguchi DoE is in fact a representation of a fractional factorial DoE, with the difference that the degrees of

freedom follow an orthogonal array in its set-up. However, in its most simple form, such as the Taguchi L4, its configuration is no different from a fractional factorial 2³⁻¹ design. Figure 1 shows a schematic of the experimental space, and the location of the design cases employed during this study.

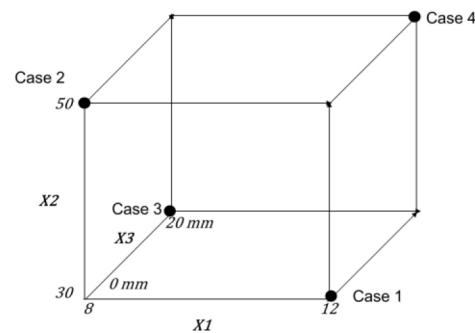


Figure 1. Taguchi DoE experimental space.

The Taguchi DoE was used to identify the impact of three mixer design factors - number of blades, angle of blades and distance from the injector - on the performance of an SCR system, more specifically NH₃ UI, Midcone pressure drop and Wall film formation. In total four cases were run with the design configurations as shown in Table 1.

Table 1. Parameters for the Taguchi DoE.

Case	Blade number	Blade angle	Distance
1	12	30°	0 mm
2	8	50°	0 mm
3	8	30°	20 mm
4	12	50°	20 mm

Confounding

One drawback of the L4 Taguchi DoE set-up, is its inability to capture 2nd order interaction due to confounding of signals between factors [12]. Thus, in the current set-up it is not possible to completely assert that the impact of a factor is in fact the result of such factor, or the interaction between two factors (confounding). For the Taguchi L4 DoE there are three possible confounding e.g. the impact of factor X1 could also belong to the interaction of factor X2 and X3 (Table 2). However, it is known that higher order effects are very seldom significant [12]. Therefore, it is assumed that main effects - e.g. X1, X2, X3 - are indeed the factors of impact.

Table 2. Possible confounding cases for Taguchi L4 DoE.

Case	X1	X2	X3	X1X2	X1X3	X2X3
1	+	-	-	-	-	+
2	-	+	-	-	+	-
3	-	-	+	+	-	-
4	+	+	+	+	+	+
Confound	1	2	3	3	2	1

Linear Regression

The results of an experiment - assuming that its outcome is dependent on experimental conditions - can be defined by a function of the experimental variables [13]. A first order response can be approximated from the Taguchi L4 DoE by a linear regression function of the form:

$$Y = \beta_0 + \sum_{i=1}^k \omega_i x_i + \varepsilon$$

Equation 1

Where factors $\omega_{i...k}$ and $\beta_{0...k}$ are regression coefficients, x_i is the independent variable, and ε is the estimated error [10], [11], [12]. Due to the linear nature of the polynomial function in Equation 1, the regression model is limited at predicting linear behaviors only, thus, in the case of complex and nonlinear phenomena, the reliability of the regression model will be challenged. Moreover, it is impossible to determine optimisation points (apart from the maximum and minimum within the experimental space); to do so, it would be necessary to implement a quadratic model capable of detecting inflection points. However, quadratic optimisation is a topic for future work and is not the aim of this study. The linear regression model here presented can be used as a design tool, akin to a performance map, that will help the designer navigate towards the desired output of the system.

Geometry Setup

In order to represent the typical configuration for light duty vehicles, the three-dimensional SCR system models used for this study consisted of a DOC (Diesel Oxidation Catalyst), a medium cone, an injector, a turbine styled static mixer in a variety of designs according to the DoE, followed by an SCRF (Selective Catalyst Reduction Filter); moreover two extruded volumes - at beginning and end of geometry - were added in order to ease the simulation process. Figure 2 shows the domain of the internal volume for CFD analysis.

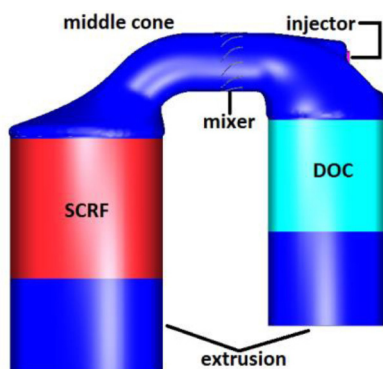


Figure 2. Internal model for CFD analysis.

The study herein, assessed the impact of three geometric factors, (X1) mixer blades number, (X2) blades angle and (X3) distance between injector and mixer, on the performance of three SCR system outputs: NH_3 UI, Midcone pressure drop and Wall film formation. Each geometric factor was modified at two levels (minimum and maximum point). The factors and levels considered in this study were

established based on manufacturing capabilities for mixer components. Figure 3 depicts the geometric parameters under evaluation.

Mesh

A finite volume spatial discretization was performed using the commercial software AVL-Fire Fame Hexa 2014 version. The mesh was developed with a combination of hexahedral and tetrahedral components (hybrid mesh). The domain used a 4 mm mesh size for discretization. Critical zones, at the periphery of the mixer blades, were refined with a level of 0.5 mm, and heat transfer properties were captured using a three layers mesh at the wall [14]. Mesh independency was verified using the Grid Convergence Index (GCI) method by Roach [15]. Table 3 shows the number of cells contained for each mesh.

Table 3. Mesh cell number for Cases on Taguchi DoE.

Case	Mesh cell number
1	549,883
2	313,201
3	311,065
4	822,055

CFD Setup

All the simulations in the study were performed with the commercial software AVL-Fire Workflow Manager 2014, using the following modules: Porosities, General gas phase reactions, Species transport, Wall film, Thin walls and Spray. The simulations were considered as a multiphase phenomenon in transient state with $\Delta t = 0.001$ sec and $\Delta t = 0.0005$ sec (during injection) with a maximum of 30 iterations per time step. The UWS was injected after the exhaust flow had fully developed inside the domain. The inlet gas, considered as compressible flow, was composed of different species typically found in exhaust gases [16].

The DOC and SCRF catalysts were treated as porous medium, where the relationship between pressure drop and velocity is settled by the Forchheimer model for multiphase calculations (Equation 2):

$$\frac{\partial p}{\partial l_1} = -\alpha_i \cdot \alpha_{rel} \cdot \mu \cdot v_i - \zeta_i \cdot \zeta_{rel} \cdot \frac{\rho}{2} \cdot |v| \cdot v_i$$

Equation 2

Where:

$\frac{\partial p}{\partial l_1}$ Pressure gradient within porous material

α_i Viscous loss coefficient

α_{rel} Relative viscous loss coefficient

μ Molecular (laminar) dynamic viscosity

v_i Local velocity

ζ_i Inertial loss coefficient

ζ_{rel} Relative inertial loss coefficient

ρ Domain fluid density

The linear and the quadratic term, respectively account for the viscous and inertial losses of the flow inside the porous medium. These loss coefficients were estimated based on the physical properties such as length, CPSI, Wall thickness and washcoat loading. The k - ϵ - f model was used for turbulence, which is a modification of Durbin's eddy-viscosity model, with the aim of improving the numerical stability of the original model $\overline{v^2} - f$ solving the transport equation using $\zeta = \overline{v^2}/k$ instead of $\overline{v^2}$ [17]. The walls were treated as adiabatic, imposing a non-slip condition except for the catalyst walls. Table 4 shows the exhaust boundary conditions used during the study.

Table 4. Boundary conditions on the exhaust system.

Boundary condition	Parameter
Exhaust mass flow	168 kg/h
Exhaust temperature	340°C
Static outlet pressure	1415 Pa

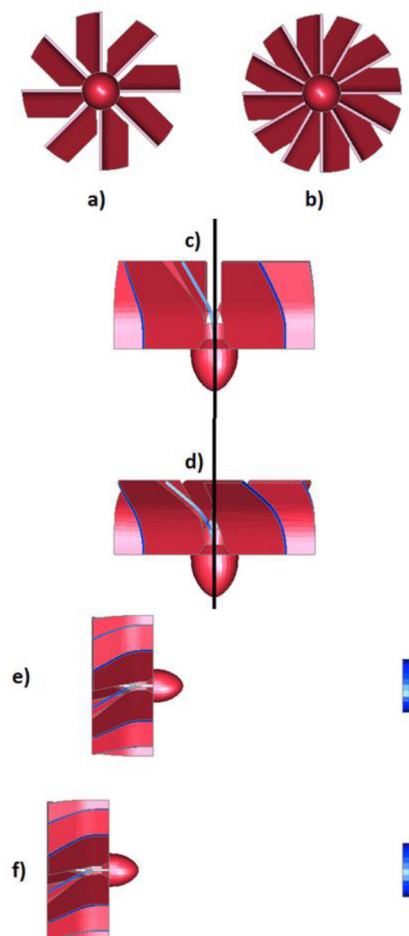


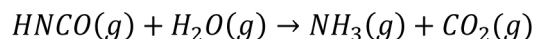
Figure 3. Factors and levels considered for the study. Mixer: a) 8 blades. b) 12 blades. Angle: c) 30°. d) 50°. Distance between injector and mixer: e) 100 mm. f) 120 mm.

Spray calculations were based on a statistical method referred to as the Discrete Droplet Method (DDM). Lagrangian trackers were used to follow the UWS droplets through the computational grid [18]. Full two-way coupling (interaction) between the gas and liquid phases was taken into account. A solution of 32.5% urea and 67.5% water was considered for the calculation of UWS injection [19][20]. UWS was dosed in standard amounts (α), described as feed ratio, typically applying a stoichiometric amount ($\alpha = 1$). The subsequent generation of NH_3 in the hot exhaust gas is carried out in three steps [21]:

1. Evaporation of water.

$$(\text{N}_2)_2\text{CO}(aq) \rightarrow (\text{NH}_2)_2\text{CO}(s \text{ or } 1) + 6.9 \text{ H}_2\text{O}(g)$$
2. Thermolysis of urea into ammonia and iso-cyanic acid.

$$(\text{NH}_2)_2\text{CO}(s \text{ or } 1) \rightarrow \text{NH}_3(g) + \text{HNCO}(g)$$
3. Hydrolysis of isocyanic acid.



Hydrolysis of HNCO is considered as homogenous gas phase reaction using the coupling interface of Fire to the CHEMKIN chemistry solver [21], and applying the SCR-thermolysis evaporation model. Kuhnke model was used for the spray/wall interaction [19]. For the particle sizes, a diameter vs probability curve, using a Rosin-Raimler distribution, was fed into the solver, Table 5 shows the boundary conditions for the injection set up. The spray parameters were obtained from an injector measured with a Phase Doppler Particle Analyzer (PDPA).

Table 5. Spray parameters.

Injection parameters	Value
UWS dosing	28.8 mg/sec
Frequency	5 Hz
SMD	75
Number of holes	3
UWS velocity	22 m/sec

The uniformity index calculation used for this study was based on the uniformity index Alpha ratio (UI_α) proposed by Johansson et. al. (2008) modified to show uniformity as a percentage (Equation 3):

$$\text{UI}_{\text{NH}_3} = 1 - \frac{\sum_i |\text{NH}_{3i} - \text{NH}_{3\text{avg}}| A_i}{2\text{NH}_{3\text{avg}} A_{\text{total}}} \times 100$$

Equation 3

Where NH_{3i} is the Ammonia in cell i , $\text{NH}_{3\text{avg}}$ is the average Ammonia of all cells, A_i is the area of cell i , and A_{total} is the total area of the centre of the catalyst [22].

RESULTS AND DISCUSSION

Initial results of the Taguchi L4 DoE are shown in Table 6, it can be seen that cases 2 and 4 show the highest NH_3 UI performance, however, they also resulted in the highest pressure drop at 652 Pa and 894 Pa respectively. Case 1 and 3 did not manage to pass over 80% NH_3 UI. Pressure drop was consistently low for case 1 at 220 Pa.