

Computational Fluid Dynamics Study of Gaseous Ammonia Mixing in an Exhaust Pipe Using Static Mixers

Gianluca Padula, Philipp Schiffmann, Matthieu Lecompte, and Olivier Laget
 IFP Energies nouvelles, Institut Carnot IFPEN TE

ABSTRACT

Ever growing traffic has a detrimental effect on health and environment. In response to climate warming and health concerns, governments worldwide enforce more stringent emission standards. NO_x emissions limits are some of the most challenging to meet using fuel-efficient lean-burn engines. The Selective Catalytic Reduction (SCR) is one consolidated NO_x after-treatment technique using urea water solution (UWS) injection upstream of the catalytic converter. A recent development of SCR, using gaseous ammonia injection, reduces wall deposit formation and improves the cold-start efficiency.

The mixing of gaseous ammonia with the exhaust gases is one of the key challenges that need to be overcome, as the effectiveness of the system is strongly dependent on the mixture uniformity at the inlet of the SCR catalyst. Here a CFD modeling approach is presented to study the effects of different static mixer geometries to find the optimal trade-off between pressure-loss and ammonia/exhaust gas mixture homogeneity in a compact system, which is demonstrated on various blade mixer geometries. The effects of air and ammonia mass flow rates at different temperature conditions were investigated to identify critical operating conditions. It is demonstrated that the pressure loss over the mixer is a function of the mixer blocked area of the exhaust pipe but also of the mixer's geometrical features.

CITATION: Padula, G., Schiffmann, P., Lecompte, M., and Laget, O., "Computational Fluid Dynamics Study of Gaseous Ammonia Mixing in an Exhaust Pipe Using Static Mixers," *SAE Int. J. Engines* 10(4):2017, doi:10.4271/2017-01-1018.

INTRODUCTION

Governments worldwide are enforcing emission standards on the automotive industry to limit the extend of pollutant emissions in the context of an increasing number of motor vehicles. These standards for light duty vehicles, including passenger cars, require aftertreatment system efficiency improvements at a competitive price, with low fuel penalties in a compact packaging. The limits for light duty vehicles are currently defined by the EURO 6 legislation in the EU and by the Tier 2 standards in the USA, with a limit for Diesel vehicle NO_x emissions of 0.08 [g/km] and 0.07 [g/mi] respectively.

Different techniques for the reduction of pollutants have been proposed, each with a specific target (*i.e.* the elimination or at list the reduction of one category of pollutants). The Selective Catalytic Reduction, that has been developed since the late 1970s for industrial use, is one consolidated technique to reduce NO_x emissions [1]. The reduction is achieved by injecting a compound that forms, with NO_x , non-toxic reaction products. Ammonia is commonly used in these applications [2], because it can reduce NO_x in the presence of oxygen and does not create additional CO_2 in the reduction process, as opposed to processes where hydrocarbon based fuel is used for NO_x reduction.

A catalyst is needed to lower the activation energy for the reaction of nitrogen oxides with ammonia [1, 2, 3] to proceed, and that it selectively progresses towards creating molecular nitrogen. Due to safety concerns (*e.g.* toxicity and corrosiveness), the unstable nature of the compound, and the requirement of pressure storage containers, pure ammonia is typically not used in automotive applications. In the past years, several ammonia precursors have been analyzed, in order to find a suitable substitute for pure NH_3 . These substances can be divided into two main groups: liquid ammonia precursors and solid ammonia precursors. The liquid precursors are usually made using a water solution (UWS) of a chemical species that can release ammonia at high temperatures. UWS commonly used in trucks and heavy duty vehicle applications are marketed under the trade names AdBlue or Diesel Exhaust Fluid (DEF). The solution is typically composed of 32,5% urea and 67,5% of water. The release of ammonia from UWS takes place in a three-step-process [4]: water evaporation, urea thermolysis and isocyanic acid hydrolysis. This process requires a high activation-temperature, since the first release of ammonia begins after the water evaporation (generally over 130°C) [5]. The evaporation of water requires a lot of enthalpy from the exhaust gases, reducing the system effectiveness during cold start. On the other hand, this precursor has its freezing point at -11°C, which is not sufficient to keep it from freezing in colder climates. Consequently, an additional heating system is required. Other liquid compounds have been proposed to increase the content of ammonia, like

guanidine salts [3]. However, as pointed out by Kröcher et al. [2] and Fulks et al. [5], the liquid precursors are prone to similar problems: low NH_3 content, high activation temperature, low freezing point, and wall film deposition. In addition, during several tests a deposit formation has been observed, due to cyclic heating and cooling. Some authors [6,7] observed that improving the atomization of the injected precursors, reduces some of the problems due to faster evaporation. However, deposit formation and NH_3 stratification at the catalyst inlet are remaining problems. This last point increases the cost of the system as the catalyst needs to be longer to increase its NH_3 storage capabilities and avoid ammonia slip.

To overcome the difficulties with liquid ammonia precursors, also solid reductants have been proposed, as for example, ammonium salts and metal amines [5]. The main advantage of these solid reductants is the increased ammonia density. For example to convert 1g of NO_x , four times less volume is required when using ammonium carbamate instead of UWS [8]. In addition ammonium salts improve the cold-start behavior compared to UWS, due to its lower activation temperature [5,9]. Another advantage of solid reductants is that NH_3 is released [10,11] in a solid to gas transition without formation of a liquid phase, avoiding the problem of wall film and deposit formation.

One problem with injecting gaseous ammonia to the exhaust is mixture stratification. A uniform ammonia distribution is required in front of the catalyst surface, to maximize the NO_x conversion efficiency of the SCR system. From experimental observations of radial mixing in a pipe, a mixing length of 50 to 100 pipe diameters is required for homogeneous mixing to occur naturally [12]. The introduction of static mixers reduces this mixing length by increasing the eddy diffusion as one of the driving mixing mechanisms [12].

The use of static mixers has been proposed in several applications, especially related to processes used in the chemical industry [13]. Some authors proposed and tested some mixers for AdBlue, from the Venturi mixer design by Kowatari et al. [6] or by Nishioka et al. [14] to the Bluebox system proposed by Alano et al. [15]. However, as pointed out by Zheng et al. [16] the use of a static mixer with AdBlue is extremely dependent on the application, since its shape, length and efficiency are affected by engine speed, load, and operating temperature. UWS mixer need to serve a dual purpose, not only do they need to contribute to the mixture uniformity upstream of the catalyst, but they also need to improve evaporation of the UWS by droplet/wall interaction, in order to favor the release of ammonia [17].

This work focuses on the process of developing the little investigated gas/gas mixers in an automotive aftertreatment system. These mixers can be decisively different from liquid/ gas mixers as their sole purpose is to maximize the mixture homogeneity at the SCR catalyst inlet. The effects of different static mixer geometries on the mixing

characteristics of air with gaseous NH_3 are studied, in order to find the optimal trade-off between pressure-loss and ammonia distribution uniformity in a compact system. To achieve this goal the effects of

- Different injector geometries,
- Temperature and NH_3 concentration,
- Blade mixer design variations,
- Converging mixer design iterations,

were investigated. This study contributes to the methodology of injector and mixer design development, presented here with the example of blade mixers. Moreover, it helps to identify the critical design points (high flow rates and high temperatures) which show the highest amount of mixture stratification.

NUMERICAL METHOD AND TURBULENCE MODEL

A correct estimation of the turbulent viscosity and the turbulent dissipation is crucial for the correct estimation of the mixing characteristics, especially in the presence of the static mixer. In their numerical simulations on mixers Zhang et al. [18] use a standard k- ϵ model. However, a systematic underestimation of the ammonia homogenization in the CFD simulations is observed compared to experimental results, as pointed out by Fisher et al. [19]. They state that the use of a Reynolds stress model (RSM) could reduce the underestimation of the ammonia uniformity, since it takes into account the anisotropy of the Reynolds stress tensor. The approximation made in the calculation of the turbulent dissipation, that is directly affected by the isotropic assumption, has a strong impact on the droplets dynamics of a coupled Euler-Lagrange approach. However, they also observe that this model increases the computational effort by about 20%, if compared to k- ϵ model, without completely eliminating the underestimation in terms of uniformity. Zöchbauer et al. [20], made similar observations of an underestimation of mixture homogeneity for a static swirl-mixer. By tuning the Schmidt number the RSM prediction of the turbulent structures and as a consequence the mixing representation could be improved [21]. It needs to be pointed out that the velocity field calculation is in agreement with the measurements for all the different turbulent models and that the underestimation of the uniformity index is related only to underestimated turbulence intensity and turbulent mixing.

In this study the commercial CFD code ANSYS Fluent 15.0 is used to solve the 3-dimensional turbulent flow using a steady state RANS approach, with the Realizable k- ϵ model and enhanced wall treatment. This model provides a new formulation of the turbulent viscosity (ν_t) and a modified formulation for the dissipation rate (ϵ), which improves the accuracy of the standard k- ϵ model in regions where flow features include strong streamline curvatures, vortices, and rotations.

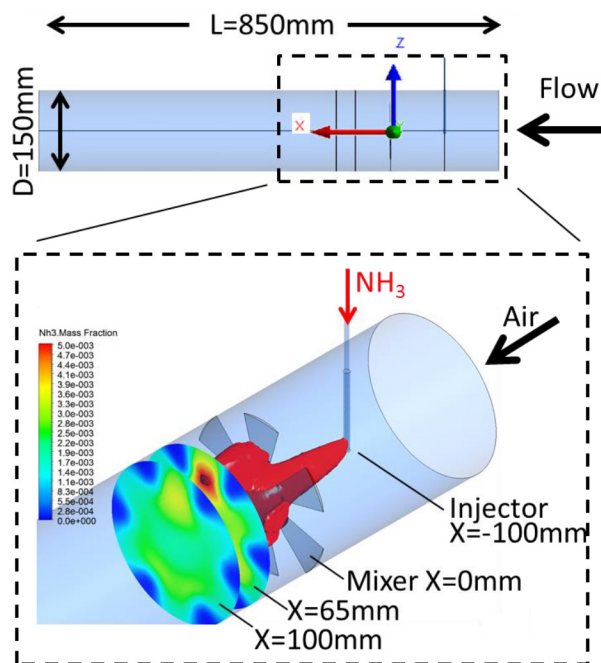


Figure 1. Tube topology, with the indication of the sections used for evaluating the mixture homogeneity.

The model uses gaseous ammonia vapor (NH_3) which is injected into the main air flow. Air instead of a more realistic exhaust gas mixture is used in anticipation of future validation experiments in an optical exhaust test bench. Indeed, in the experiments air is preferred for cleanliness, increased simplicity of the setup and for health risk reasons. The validation of the results, with the comparison of different turbulent closures, will be conducted in future studies on a dedicated experimental test bench [22].

NUMERICAL SCHEMES

The numerical scheme adopted in Fluent for the pressure-velocity coupling is the SIMPLE algorithm. For pressure, density, momentum and specie transport a second order upwind scheme is adopted, while for turbulence kinetic energy and turbulence dissipation a first order upwind scheme is chosen.

GEOMETRIES AND MESH GENERATION

The pipe considered has a diameter (D) of 150 mm and a length (L) of 850 mm, resulting in a $L/D \approx 7$ providing the base for good numerical accuracy and stability. The tetrahedral mesh is obtained with the ANSYS Meshing tool. It is carefully refined near the pipe wall and mixer surfaces. The thickness of the first two layers of the mesh is imposed evaluating the non-dimensional wall distance y^+ , to properly capture the viscous sublayer, through the log-wall law [23]. Figure 1 shows a sketch of the pipe-injector-mixer topology. The mixture homogeneity is monitored in two sections located at 65 and 100mm downstream the mixer. A catalyst is purposefully not included in the models, because it will reduce optical access in future stratification measurements used to be compared with the numerical results presented here. It is understood that a catalyst downstream of the mixer could affect the flow, especially in recirculation regions, and will be subject to future studies.

MESH CONVERGENCE STUDY

A mesh independence study has been performed aiming at minimizing mesh effects on the results at a minimal computational cost. The study has been conducted with the “6 blades with disk” mixer, comparing 4 different meshes with different number of cells (see Table 1). The same local refinement on injector and mixer surfaces has been adopted in all cases. The evaluation of the results is made considering pressure, velocity, Turbulent Kinetic Energy (TKE) and turbulent eddy dissipation along the pipe axis are shown in Figure 2.

Table 1. Size comparison of the meshes used for the independence study. All the dimensions are in [m].

Mesh name	Initial	Large	Medium	Fine
Minimum size	2e-3	8e-4	8e-4	8e-4
Maximum face size	4e-3	4e-3	2e-3	2e-3
Maximum size	8e-3	8e-3	6e-3	4e-3
Total number of cells	2.9M	3.7M	4.5M	7.9M

Only the first mesh shows overall significant difference in pressure compared to the fine mesh. Although also the medium and coarse mesh show some minor discrepancies compared to the fine mesh, the additional computational cost does not justify the accuracy benefit, such that from here on the “large” mesh setup is chosen, as it provides good orthogonal mesh quality with an acceptable simulation time.