Alignment of Simulation Methodology and Measurement Techniques to Predict the HC-Distribution at Catalyst Inlet for Exhaust Fuel Injection

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ABSTRACT: Injection of fuel into the exhaust system is used to support the operation of exhaust gas aftertreatment systems. When injecting a fluid into the exhaust system, one major challenge is to design the exhaust system for optimal fuel distribution and to define an appropriate injection pressure. Simulation techniques are a suitable measure to support the corresponding development process. Hence, the project “Exhaust Fuel Injection” was initiated. Project target is the alignment of simulation methods and measurement techniques to predict the HC distribution in radial and axial direction at the inlet of a catalyst. This includes the definition of suitable measurement techniques to determine the hydrocarbon concentrations upstream of a catalyst. Transient 3D Computational Fluid Dynamics (CFD) simulation was used to model the fuel injection into a purpose-built exhaust system. The simulation results of the distribution of hydrocarbons at catalyst inlet in radial and axial direction are compared with measurements performed at an engine test bench. In total 18 variations were simulated and measured and twelve of them showed deviations in the uniformity index (UI) below 2 %. Only two variations resulted in deviations in UI above 3 % . The trends in axial distribution showed good correlation between test bench and simulation. Especially the influence of injection pressure and operating point was predicted well by the simulation.

KEY WORDS: heat engine, post treatment system, fuel injection, computational fluid dynamics [A1]

1. Introduction

Continuously decreasing emission legislation limits as well as changing emission test cycles (1,2) require a significant enhancement of the exhaust gas aftertreatment functionalities. In addition to commonly used approaches to reduce nitrogen oxides (NOx), new techniques are continuously being developed and tested. One of these newer methodologies is the injection of fuel upstream of a NSC (NOx Storage Catalyst) to extend the effective exhaust gas temperature range for the NOx reduction (3). This approach as well as other technologies like urea injection for SCR (Selective Catalytic Reduction) catalysts or fuel injection for an active regeneration of a DPF (Diesel Particulate Filter), requires more attention to the design of the exhaust system. Whenever a fluid is injected into the exhaust system, ensuring equal distribution on the surface of the catalyst (high uniformity index) is one of the major challenges regarding the performance of the system. Moreover, for an exhaust fuel injection upstream NSC, the peak shape in axial flow direction at catalyst inlet has to be taken into account.

3D CFD simulations, which model the exhaust gas flow as well as the fluid injection, are a common tool to design and optimize the layout of the exhaust aftertreatment system. To enable further investigations using 3D CFD simulation on the topic of fuel injection, the most important phenomena - especially regarding spray break-up and wall film formation - need to be understood and modeled. Within the scope of this research project, it is intended to find a suitable alignment of the simulation methodology and measurement techniques to predict the hydrocarbon (HC) distribution at the catalyst inlet. It is not intended to find an optimized layout for the exhaust system, because a modified system from the common exhaust system was used. One project target is to find out which measurement technique is best suited to evaluate the HC distribution.

The fuel distribution is evaluated by the axial and radial distribution. While the radial distribution can be quantified with the uniformity index (UI), the axial distribution is characterized by the HC-concentration peak over time, as depicted in Figure 1.

![Fig. 1: Axial and radial distribution.](image)

The UI is defined as follows:

\[ UI = 1 - \frac{c'_{\text{avg}}}{c_{\text{avg}}} \]

With:
- \( c' \): standard deviation of concentration
- \( c_{\text{avg}} \): average concentration

The exhaust system designed for this project has to fulfill different requirements: (1) providing access for the measurement techniques and (2) enabling easy change of hardware variants. The
system needs to be as realistic, i.e. as close as possible to systems found on modern engine applications. The HC concentration should be analyzed via optical measurements as well as concentration measurements at different positions upstream of the catalyst brick. To align the simulation model with fired engine test results, suitable measurements are conducted on an engine test bench along with supporting 3D CFD simulations throughout the entire project.

In the first step, steady state simulations are used to evaluate the feasibility of the exhaust system design. In a next step, transient 3D CFD simulations are performed with the final exhaust system design to define a test matrix for the initial engine test phase. After completion of the first engine test phase, the measured variations on the test bench are simulated for comparison.

2. Project Approach and Boundary Conditions

2.1. Design of the Exhaust System

In order to perform a comparison and alignment of measurement and simulation, an exhaust system was designed to meet requirements regarding installation flexibility and optical accessibility for HC-measurement. The flexibility is needed to perform the parameter variations. The designed system is depicted in Figure 2. The pipes from turbocharger outlet to the bigger pipe containing the catalyst have an inner diameter of 40 mm, the radius of the pipe with the injector was varied in previous steady state simulations and found to be sufficient for flow conditions at approx. 80 mm. The mixing length for the injected fuel is comparably long to provide the possibility to vary the mixer position significantly. A second pipe is inserted (marked blue in Figure 1) which can be easily replaced with pipes including two different mixer types in three different positions. This pipe, which can contain the mixers is 250 mm long, while the distance from the injector to a mixer in top position is approx. 70 mm, to the middle positioned mixer approx. 185 mm and to the bottom position approx. 280 mm.

There are two accesses for the optical measurement, one for the endoscope perpendicular to catalyst inlet and the second one to set up the laser sheet in front of the uncoated catalyst brick. The distance between the endoscope access and the catalyst inlet is 100 mm. The catalyst brick has a diameter of 100 mm and the pipe of 119 mm to install the brick with a mat. While comparison between simulation and experimental measurement requires the same geometry, these installations were also modeled in the simulation.

The two mixer designs as well as the three different positions in which they can be mounted are shown in Figure 3.

Fig. 2: System design including optical accesses for laser and camera and providing flexibility regarding mixer type and position.

Fig. 3: Designs of the two mixers, which were used, and the possible installation positions.

For the hydrocarbon measurement downstream of the catalyst brick, a specific flange (see Figure 4) was built with probe tubes in 13 different positions, which guide the exhaust gas firstly to a valve and afterwards to a dilution tunnel where the HC concentration was measured using a fast Flame Ionization Detector (FID). The lines were heated to 220 °C to avoid any condensation of the fuel.

Fig. 4: Flange for hydrocarbon measurement downstream catalyst and set up on engine test bench.

The injector is a six hole injector with flow rates between 3 – 17 g/s with injection pressures from 5 – 200 bar. For all tests and simulations, n-dodecane (C_{12}H_{26}) was chosen as a surrogate fuel.

2.2. Simulation Approach and Definition of Variation Parameters

Before any test bench activities were started, transient simulations were performed to investigate which parameter variations lead to significant changes in the uniformity or the HC peak shape. A test matrix for simulation and measurement was set up using the results of those pre simulations. The simulations were performed with the STAR CCM+ code by cd adapco (SIEMENS) as transient simulations. The following figure depicts the most important effects, which are modeled in the simulation.
The following settings were chosen in the model:

- Polyhedral mesh with prism layer for boundary layer, conformal mesh at solid boundary, cell refinement in injector spray cone
- Ideal gas, non-reacting
- Realizable k-Epsilon Turbulence Model
- Langrangian Multiphase for modelling fuel droplets
- Liquid properties from Dodecane
- Bai-Gosman Wall Impingement
- Reitz-Diwaker Breakup
- Drag Force (Drag Coefficient → Schiller Naumann)
- Droplet Evaporation (Sherwood Number → Ranz Marshall)
- Fluid Film shell surface along with multiphase interaction with gas and droplets
- Conjugate Heat Transfer (gas – solid, liquid – gas, liquid – solid)
- Two-Layer All y+ Wall Treatment

Based on these model settings, the preliminary simulations for the evaluation of parameter significance were prepared. The following table shows the results of the preliminary simulations, showing the significant variation parameters.

Table 1: chosen variation parameters including their variation range for final test matrix.

| OP1          | OP2          | OP3          | OP4          |
|--------------|--------------|--------------|--------------|
| Exhaust temp./ mass flow | 340°C / 70kg/h | 470°C / 100kg/h | 365°C / 270kg/h | 545°C / 340kg/h |
| Injection duration | 1ms          | 1ms          | 1-2ms        | 1-7ms          |
| Injection pressure | 5bar         | 5bar         | 5bar         | 5-50bar        |
| Mixer type    | tumble / swirl | swirl        | swirl        | tumble / swirl |
| Mixer position | middle       | middle       | middle       | Top / middle / bottom |

In Table 1, the boundary conditions regarding exhaust mass flow rate and temperature for the four different engine operating points (OP) are listed as well as the corresponding ranges for the other varied parameters. With the choice of the different operating points, a wide range of exhaust temperature and exhaust mass flow rates was covered in the different possible combinations. A variation of injection duration and pressure was only possible in a range where no or a very little number of droplets occurred at the catalyst inlet. Therefore, most variations were performed in operating point 4 (OP4, high temperature and high exhaust mass flow rate).

3. Results

All parameter variations listed in the final test matrix were simulated and measured at the test bench. The following comparisons show the spatially averaged HC concentration over time and the uniformity index (UI) calculated for the 13 measurement positions (Figure 4). To evaluate the peak shape, the peak duration and the peak gradient (rising and falling edge) are compared qualitatively. The results show differences in simulation and measurement in terms of peak concentration and duration. However, the goal was to model the trends correctly when comparing qualitatively. This is discussed in the following section.

3.1. Variation of Operating Point and Injection Duration

As mentioned, four different operating points were chosen to be varied. In the two higher load points also the injection duration could be varied. Figure 6 shows the influence of the operating point with 5 bar injection pressure, 1 ms injection duration and no mixer installed.

![Fig. 6: Average HC-concentration over time for 1 ms injection duration in different operating points](image)

The measurement confirms the result of the preliminary simulations that the operating point has a big impact on the fuel distribution. The higher the exhaust mass flow rate and temperature, the higher is the concentration peak gradient and the shorter is the peak. This is due to the fact that with higher mass flow rates and temperatures, the fuel can evaporate faster and additionally is transported faster to the catalyst inlet. The general peak shape of the HC concentration can be predicted very well with the simulation, and the differences between the operating points are obvious. In addition, a variation of injection duration was measured and simulated for the highest possible injection duration in OP3 and OP4, which is shown in Figure 7. Since the injection pressure is kept constant for this variation, the increase of the injection duration results in an increased injection quantity causing a higher concentration peak. The differences regarding injection duration variation can equally be observed in simulation and measurement.
Figure 8 shows the simulated and measured uniformity indices for the different operating point variations.

The comparison of the uniformity indices (UIs) shows that the highest uniformity can be achieved in the low load operating point OP1. Overall the trend fits well and - except for one - all simulated UIs match the measured ones with only small deviations. Just the simulation in OP2 predicts an UI value which is significantly lower compared to the measurement (> 3 %).

3.2. Variation of Mixer Type and Mixer Position

Figures 9 and 10 show the simulated and measured HC concentration and uniformity results with and without mixers in different positions. As can be seen in Figure 9, a variation with mixers does not result in high differences regarding the axial distribution. But even though the differences are quite small, also in this case, the general trend is modeled well. The variant with swirl mixer in top position has the highest peak of all mixer variants, the fuel arrives faster at the catalyst inlet compared to the configuration without mixer. Regarding the UI, three of the four simulations predict the UI precisely, while for the configuration with tumble mixer in middle position, the deviation is above 3 %.

In Figures 11 and 12, the simulation and measurement results with the swirl mixer and tumble mixer in middle position for operating point 1 (OP1, low temperature and low exhaust mass flow rate) are depicted.

For the low load operating point the mixers do not have a high impact on axial distribution, which can be seen likewise in the measurement and simulation results.
The comparison of uniformity indices in Figure 12 shows first of all that the mixers could not further improve the already very high uniformity in this operating point. This can be concluded, both, from measurement and simulation.

3.3. Variation of Injection Pressure

A variation of the injection pressure was only reasonable in the high load operating point OP4, as only in this operating point no or only a very little number of droplets occurred at the catalyst inlet when increasing the injection pressure. Accordingly, Figure 13 shows the peak shapes for injection pressures of 5 bar, 20 bar and 50 bar with the same injection duration of 1 ms without mixer.

Because the injection duration is kept constant, an increase of the injection pressure results in higher injection quantities and therefore, higher concentration peaks. The gradient of the concentration peak is steeper with higher pressures, while the peak occurs at nearly the same time for the same duration.

Even with higher injection pressures, the simulation and measurement results are comparable. This applies for both parameters, the peak shape and the UI, which can also be seen in Figure 14. As observed before, the high concentrations are overestimated, while the low concentrations are underestimated by the simulation. Comparing peak duration and gradient, the simulation matches well.

3.4. Overview of Results

A summary of the measured and simulated variations can be found in Table 2.
The results can be summarized as follows:

- The general trend of the measured results for different parameter variations is matching well with the simulation results.
- Simulations with boundary conditions of operation point 1 (OP1) and OP3 (low temperature and low mass flow and low temperature and high mass flow) with and without mixers show very good correlations regarding UI. Moreover, the peak shapes match well with the measurements.
- Differences in the UI can be found in both simulations with the boundary conditions of OP2 (high temperature and low mass flow), where also the peak shapes deviate slightly from the measurements.
- Most parameter variations were simulated and measured with the boundary conditions of OP4 (high temperature and high mass flow) of which only the variation with a tumble mixer showed an unsatisfactory correlation ($\Delta UI > 3\%$).
- The influence on the peak shape of the variation of injection pressure is modeled well, while $\Delta UI < 2\%$ in two from three points.
- Deviations above 2\% and low correlations regarding peak shape can be found in some of the parameter variations with mixers. For those variations, an improved modelling of the different wall film - wall, wall film - droplet and droplet - wall interactions is needed. However, the results showed $\Delta UI < 3.6\%$ for all variations.

**5. Conclusion**

In the research project "Exhaust Fuel Injection", the hydrocarbon concentration upstream catalyst was measured and simulated using a purpose-designed exhaust system.

In this paper, the comparison of measurement and simulation results from the final project phase are presented.

Different impacts on the axial and radial distribution from the variation parameters were found. The operating point and the injection pressure had a strong influence on both, the radial and axial distribution, while the low load operating point (OP1) showed the best UI with 96\%. Increasing injection pressures increased the UI as well. The mixers had no significant impact on the axial distribution but showed an improved uniformity in the high load operating point (OP4). Overall simulation and measurement show a good correlation regarding peak shape (axial uniformity) and range of radial uniformity index (UI). Thus, a reliable alignment between measurement and simulation was achieved. However, the parameter variations with mixer did not correlate as well as the ones without mixers.

In this project, a detailed comparison of measurement and simulation of exhaust fuel injection was performed. The influence of different parameters was investigated and the significance of the various interactions of the wall film were found. To gain additional knowledge, further research work should focus on detailed measurements including wall film measurements.

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