Impact of multiple injections on adBlue Spray Decomposition in a SCR-like system using Large Eddy Simulation

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Abstract
In the present paper, numerical investigations of the adBlue injection are reported in a SCR-like system using Large Eddy Simulation (LES) based on a WALE subgrid-scale model. Thereby, the influence of multiple injections on both, the thermal decomposition of adBlue spray and the urea SCR reduction performance is especially assessed. The spray module relies on a Eulerian-Lagrangian approach and includes phenomena, like spray atomization, multi-component droplet evaporation and film deposition. The chemical reaction kinetics is described by a global mechanism of urea thermolysis and hydrolysis. Applying an uniformity index of scalar field in transient operating conditions, the impact of two different urea injection frequencies is analyzed. The results demonstrate that: (1) injection frequency affects strongly the investigated processes and quantities such as, spray evolution, mixture fraction, temperature field and NH_3 conversion; (2) adBlue deposition on SCR duct wall is a critical parameter which further affects these processes. This is, in turn, regulated by injection frequency. The suggested uniformity index provides information about the phenomena related to airborne adBlue spray and wall deposited mass. It turns out, that the multi-injection with higher frequencies seems to be favorable in getting continuous conversion and uniform distribution of NH_3 and in minimizing the adBlue deposition.

Keywords
Multiple adBlue injections, LES, Eulerian-Lagrangian approach, thermal decomposition, conversion efficiency, deposition.

Introduction
Selective Catalytic Reduction (SCR) has become the technology of choice to control the NOx emission to meet stricter environmental regulations for transport applications (cars, ships, trucks, etc.) in modern lean-burn engines. In a typical SCR system, the DEF(diesel exhaust fluid) which is mixture of 67.5 wt% urea and 32.5 wt% water commercially known as adBlue is injected in controlled fashion into the hot engine exhaust stream based on engine loading conditions. With the help of exhaust gas heat, the urea is dissociated into gaseous ammonia (NH_3) by evaporation and thermal decomposition. Subsequently, this NH_3 reacts with the NOx and converts it into harmless compound that can be finally released to the environment. Thereby, the performance of SCR system is often critical in dealing with the available space in automobile. Therefore, adBlue injection dynamics, spray evolution, thermal decomposition and mixing as well as NH_3 homogeneous distribution over the monolith entrance cross-section need to be well controlled in order to achieve a best efficiency for NOx reduction. All these processes are inherently highly transient in nature and demand adequate consideration of appropriate resolution in both time and space once relying on numerical investigation. Detailed reviews can be found in [1, 2, 3, 4].

It is worth noting that the main issues which are maximizing NOx reduction performance and minimizing ammonia slip as well as formation of deposits [5] are hard to tackle because of the two subtle limiting factors, namely incomplete urea decomposition in the SCR system and non-uniformity of ammonia (NH_3) over the monolith entrance cross-section. These limiting factors are attributed to both the injection system and the interaction of the adBlue spray with the hot-gas cross-flow and SCR wall. Since the injection process obviously determines the initial conditions for reactions and catalysis, it is essentially responsible for optimal operation of selective catalytic reduction (SCR) systems. In order to highlight the influence of various adBlue injectors along with injection parameters, like injection timing and injection pressure, on spray dynamics, both experimental and numerical investigations have been primarily and largely carried out [6]. Recently, the effect of hot cross-flow rate and temperature on the spray dynamics within the SCR system has been reported [6, 7]. Thereby, the presence of a hot gas flow inside the channel drags the adBlue droplets towards the outlet, while influencing the droplet spray distribution. In particular, smaller droplets are more susceptible to be transported along the carrier gas, while the bigger droplet having more momentum will withstand the cross-flow and impinge on the SCR wall. These studies are aimed solely at adBlue spray dynamics in a generic SCR system, a very little attention is paid on optimal SCR-design for NOx reduction efficiency and performance output.

Regarding the spray-wall impingement, it is a well known fact that, a liquid wall film is formed when the wall temperature is below the Leidenfrost temperature. This film evaporates and, because of the resulting enthalpy of evaporation, causes increased local cooling of the wall. In addition, the liquid film flows downstream along different regions of wall temperatures. Therefore, it features a wide-ranging spray-wall interaction regimes on hot wall and liquid film, namely; film formation, spray rebound, breakup and splashing [8]. Based on wall temperature the adBlue film can further leads to formation of urea and by-product deposition [5]. Brack et al. [9] suggested a reaction mechanism that helps to calculate the chemical composition of the deposits in dependence of the film temperature, residence time and thickness of the wall film (see, [5]). It is worth noting that the formation of deposits can lead to the failure of the dosing strategy; in turn a failure of SCR system by clogging the exhaust pipe or, at least, increasing the pressure drop.

In the perspective of numerical modeling and analysis, RANS based methods are preferred to describe the carrier phase turbulence owing to its low computational cost. Despite the fact that processes in SCR system are highly unsteady and complex contributions of LES in SCR systems are very rare [10, 11, 12, 13]. In fact Ström et. al. [11] clearly pointed out the impact of turbulence models in predicting the transition of turbulence to laminar flow in honey-combed SCR. Moreover, Kaario at al. [13] specifically reported that the evaporation and unsteady mixing phenomena can only be represented by LES or hybrid LES-RANS models. For the first time LES study has been recently performed by Nishad et al. [10] to analyze the spray dynamics resulting from an adBlue sprayed from a six-holes circular orifice injector into a hot gas cross flow inside a square channel. This configuration corresponds to the experiments by Spiteri [6]. In the present contribution, the spray module designed in [7, 10] is used. It relies on an Eulerian-Lagrangian approach within the LES framework under consideration of two-way coupling between both gaseous and liquid phases. It includes the required sub-models (e.g. atomization, multi-component evaporation, spray-wall interaction etc.) to find out the effect of multi-injection on adBlue spray decomposition and deposit formation. For the unsteady description of the turbulent carrier gaseous phase, the wall-adaptive local eddy-viscosity (WALE) subgrid scale (SGS) model is employed to close the SGS stress tensor in the filtered equation of momentum, and a gradient assumption for the SGS scalar flux vectors in the filtered scalar governing equations. A Lagrangian droplet tracking is followed to retrieve the evaporating adBlue droplets produced by the atomization of liquid jet. Especially the primary and secondary breakup models including an advanced collision model are considered to account for the atomization generated by the multi-hole circular orifice injector used. To describe the heat and mass transport process within and from the droplet a well-proven multi-component droplet evaporation model is incorporated.

In the present paper, this Eulerian-Lagrangian based LES methodology is extended for thermal decomposition of urea in the gaseous phase, where, depending on how the heat of thermal decomposition of urea is accounted for, while the deposits can be formed due wall-film development during spray-wall impingement. For this purpose, an evaporating wall-film modeling is integrated. This extends the approach suggested by O'Rourke et al. [14] by accounting for the rebound in addition to classical drop splashing and breakup [8]. Note that in the case of droplet deposition, impacting drops and wall-films are treated as so-called wall particles. For these conditions, 2-D evaluation equations for mass, energy and momentum conservation are solved for wall film using these wall particles [14].

The objective of the present paper is thus to investigate the relevant physical phenomena in a SCR-like system, to predict and to track the conversion and deposit formation during multiple injections of adBlue. This prerequisites the development of a validated predictive tool and then recommendation of the design rules enabling to ensure a suitable NOx conversion while avoiding deposit formation to improve SCR efficiency and reliability.

Section 2 of the present paper briefly summarizes the model formulations. Section 3 provides a description of numerical set-up for providing turbulence initial and boundary conditions for hot gas flow, and strategies for adBlue injection. The achieved LES results are then discussed in Section 4. Various numerical analyses are subsequently carried out in order to point out the effect of multiple injections on both the thermal decompositions of adBlue spray and NH_3 conversion using an uniformity index of scalar field.

Model formulation

In this section, a brief overview of the adopted numerical methodology to simulate the SCR system is outlined. The Wall-adapting local eddy-viscosity (WALE) model is applied to capture the flow-turbulence with the open source KIVA-4mpi CFD code [17](Los Alamos National Laboratory (LANL), Los Alamos,NM, USA). This code is based on an arbitrary Eulerian-Lagrangian (ALE) , in which the Lagrange particle framework is used to track the adBlue spray in the SCR duct. The Kelvin-Helmholtz (KH) and Taylor-analogy breakup (TAB) model are applied to represent the adBlue injection and spray atomization processes. The adBlue evaporation is modeled using the comprehensively verified multi-component evaporation model for binary mixture of urea-water-solution [7] which is originally stemmed from [18]. Thereby, the wall/droplet interaction description relies on an advanced extension of the Lagrangian based film model suggested by O'Rourke et al. [15]. This extension includes droplet splash, film spreading due to impingement forces, motion due to film inertia, deposition, and rebound (see in [16]). The numerical simulation with LES is inherently a initial and boundary value problem. Therefore, special attentions are needed especially to set up the fully developed initial turbulence and subsequent transient inflow boundary conditions. To make this paper concise and clear, this methodology is not described here, it was already presented in the previous study [10]. Moreover the detailed validation of the adBlue injection and subsequent atomization under varied conditions were also reported in [10]. Once the injected adBlue is atomized, the subsequent evaporation and thermal decomposition of gaseous urea are accounted for by following three global mechanisms (see Eqn 1-3) namely, evaporation of urea water solution, thermolysis of gaseous urea and hydrolysis of isocyanic acid (see [7] for more details)..

$$CO(NH_2)_2(aq) \rightarrow CO(NH_2)_2(g) + H_2O(g) \tag{1}$$

$$CO(NH_2)_2(g) \rightarrow NH_3(g) + HNCO(g)\ , \tag{2}$$

$$HNCO(g) + H_2O \rightarrow NH_3(g) + CO_2(g)\ . \tag{3}$$

Numerical set-up

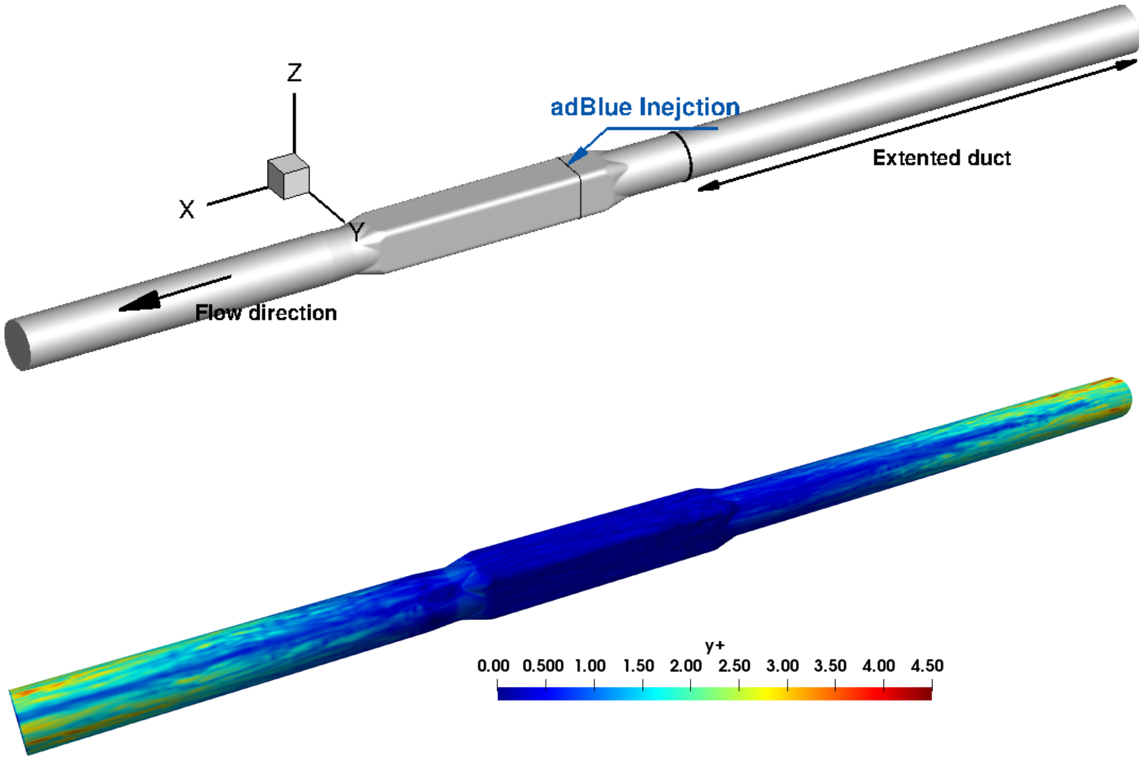

Figure 1. Computational domain with injection location (top) and the Y^+ value along the SCR duct (bottom)

In this study, the selected SCR duct (see Figure 1, top) under investigation is taken from the experimental work carried out by Spiteri [6], in which a comprehensive data-set for the numerical validation of the adBlue injection are provided. This consists of a channel with square cross-section into which 6-holes circular orifice pressure-assisted nozzle injects adBlue. The domain consists of this rectangular channel where all experimental measurement have been carried out, and of additional circular ducts which are used to provide the flow inlet and outlet. As already reported in [10], the duct is extended 10 D upstream to injection point in order to provide fully-developed LES inflow boundary conditions to the test section. This way the total length of duct is approx. 2.02 m with 80x80 mm^2 square cross section and 80 mm circular duct diameter. The hexahedral structured mesh is used to spatially discretized the whole domain with approx. 4.7 Millions control volumes. The selected operating parameters for the present study is listed in Table 1. It features a 6-holes circular orifice injector with 50° inclination to the horizontal plane. The injection duration is 60 ms for the 1 Hz case, which is splited into two 30 ms for the 2 Hz case, making the total adBlue mass injected be the same for both cases. To track the adBlue injection and subsequent spray dynamics, a total number of 480,000 computational particles (parcels) are used during the simulation. Simulations are performed on Intel® Xeon® Processor E5-2670, 32GB RAM with 16 CPUs and the graph partitioning package pMETIS is used to decompose the domain. To simulate 1 second of physical time requires aprrox. 2400 CPU-hours. More details about numerical set-up especially setting up the turbulence initialization and boundary condition are provided in [10].

Table 1. The operating parameteres

	injection frequency (Hz)	mass flow $\dot{m}_g$ (kg/s)	gas temperature T_g/T_w(K)	adBlue injection rate g/s
case 1	1 (SOI - 0 sec)	100	673	4.5
case 2	2 (SOI - 0, 0.5 sec)	100	673	4.5

Results and discussion

As pointed out earlier, a fully developed turbulent flow is initialized in the whole domain, with fully developed inflow conditions. Figure 1 (bottom) shows the accomplished instantaneous Y^+ along the SCR duct wall for this configuration with $Y^+ < 1.0$ ($\approx$ 120 μm) in rectangular measurement section, which is important in order to carry out wall-resolved LES. It should be noted here that the calculated Y^+ is based on only gaseous flow without adBlue injection. The adBlue injection results in film formations on the SCR duct which further develops especially during consecutive injection.

The LES is then carried out with respective adBlue injection (e.g. 1Hz, 2Hz injection frequencies) for 1 second in order to evaluate the influence of multi injection (case 2) against single injection (case 1). The instantaneous velocity profile and droplet distribution profile along the part of duct length is shown in the Figure 2 for SOI 75 ms. Since all the adBlue is already injected in the case 1 by this time, comparatively more dense pockets of adBlue spray is clearly visible as compared to case 2. The influence of higher mass loading is also visible in overall NH_3 conversion (see Figure 3) and carrier phase temperature (see Figure 4). Since, the SCR duct dimension is relatively small, most of the injected adBlue impinge on the wall resulting in a complex spray-wall impingement phenomena, and subsequent film formation. As expected, heavy deposition of adBlue droplet is observed for the case 1 due to higher mass loading and respective influence of evaporation, $NH-3$ conversion and thermal profile can be seen in Figure 2-4. This adBlue film then moves slowly due to shear flow along the film surface and impingement pressure while simultaneously undergoing phase change (evaporation, thermal decomposition etc.) processes. A high degree of non-uniformity is clearly visible from results, as evaporation and conversion dynamics are dominated in lower wall region. Figures 5-7 represent the snapshots of spray, NH_3 and gas temperature at 550 ms. At this instance the second injection in case 2 is just completed. The influence of second injection on overall profile for spray, NH_3 and gas temperature is clearly visible in case 2. While, in case 1 all the airborne droplets are already convected through the outlet, the visible influence on NH_3 conversion and gas temperature is purely from the adBlue wall-film dynamics. Thereby, the available heat in the exhaust gas has not been utilized and additionally most of the exhaust gas get away without being reduced. It should be noted here that this configuration provides evidence that, using LES it is possible for specific engine loading and exhaust flow (flow rate, temperature, NOx level) injection rate with various frequencies can be achieved for SCR systems.

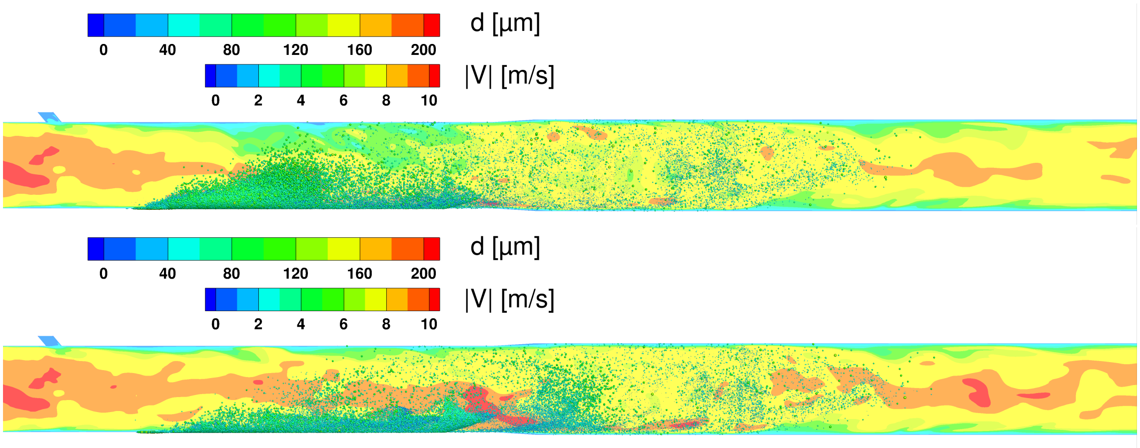

Figure 2. Comparison of spray and velocity profile at 75 ms after SOI for case 1 (top) and case 2 (bottom)

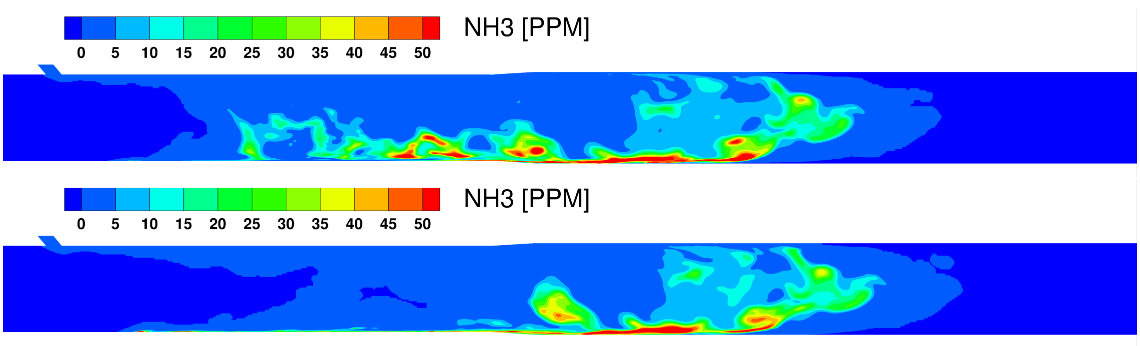

Figure 3. Comparison of NH_3 conversion at 75 ms after SOI for case 1 (top) and case 2 (bottom)

To get further insight into the mixing process within the SCR duct, a Coefficient of variation (CoV) is defined which is generally used as measure of uniformity in a pipe/duct cross-section. It is expressed as a standard deviation

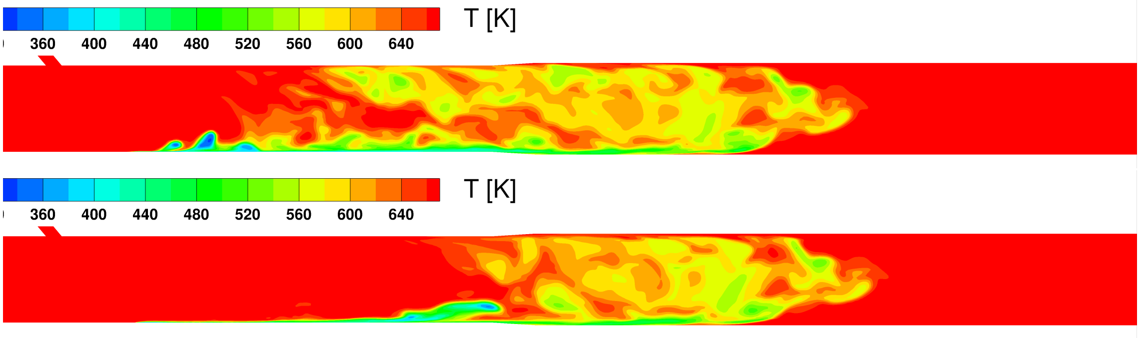

Figure 4. Comparison of temperature evolution at 75 ms after SOI for case 1 (top) and case 2 (bottom)

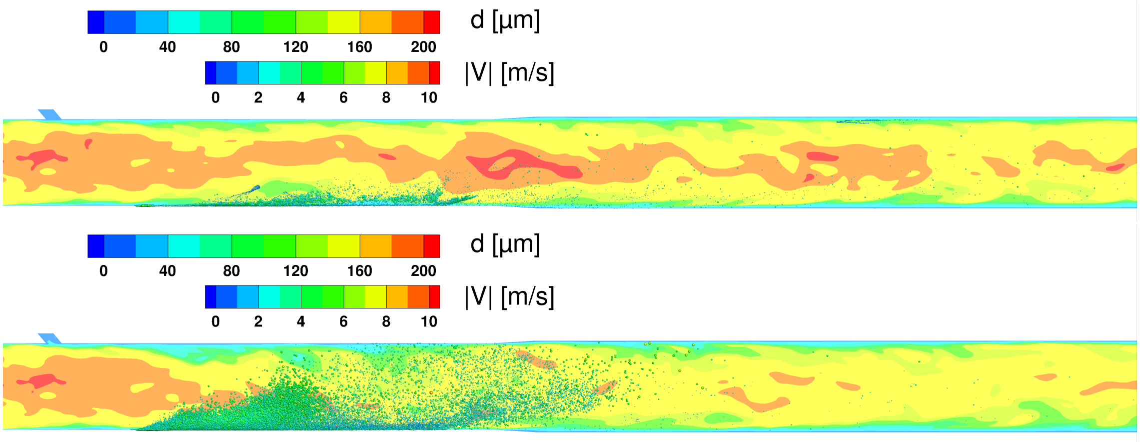

Figure 5. Comparison of spray and velocity profile at 550 ms after first SOI for case 1 (top) and case 2 (bottom)

normalized by the mixture fraction range for the whole domain and time space as given in Eqn 4.

$$CoV(X) = \frac{\sqrt{\overline{X_i X_i} - \overline{X}_i \overline{X}_i}}{max(\overline{X}_i) - min(\overline{X}_i)} \tag{4}$$

The cross sectional CoV is calculated along the duct length for 1 second of physical time as shown in Figure 8. As already mentioned before, the high degree of non-uniformity is also evident from CoV plot. The CoV shows the influence of multi-injection as visible in the case 2 (see Figure 8, right) where the conversion of NH_3 is still persistent in downstream and later stage of the spray dynamics. The two distinct physical phenomena can also be observed by looking at the CoV profile. The first one is marked by red dashed line representing the evaporation of airborne adBlue droplets and subsequent conversion into NH_3, while the second one is marked by black dashed line representing the wall-film evaporation and conversion dynamics. The later one is almost localized at the SCR duct suggesting a slow moving adBlue film. The similar trend is also visible for the CoV plot for iso-cyanic acid as shown in Figure 9.

Finally, the total mass of adBlue deposited on the SCR duct is plotted against the physical time for both cases in Figure 10. The heavy adBlue deposition is clearly visible initially for the case with single injection (case 1) as compared to case with splitted injection (case 2). The subsequent injection in case 2 further builds up the deposited adBlue which is now comparable to the case 1. However, overall case 2 still performs well as compared to case 1 in terms of less adBlue deposition. Note that, the simulation is carried out for physical time of only 1 second. Therefore, the deposited mass mostly represents the liquid film. The evaluation of solid deposition formation for long physical time is not included in this paper, and left for future work.

Conclusions

In the present study, the impact of the multi-injection of adBlue on SCR system is evaluated. It is achieved by comparing two injection frequencies, namely 1Hz and 2 Hz. The considerable difference in the system performance especially in terms of adBlue evaporation, NH_3 conversion and deposition dynamic is observed. A CoV is used to describe the degree of mixed-ness. It provides information about the phenomena related to airborne adBlue spray and wall deposited mass. It turns out, that the multi-injection with higher frequencies seems to be favorable in getting continuous conversion and uniform distribution of NH_3 and in minimizing the adBlue deposition.

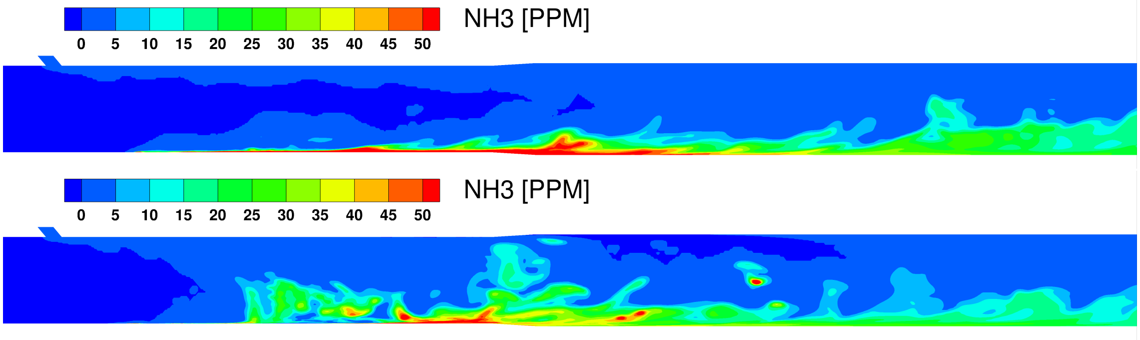

Figure 6. Comparison of NH_3 conversion at 550 ms after first SOI for case 1 (top) and case 2 (bottom)

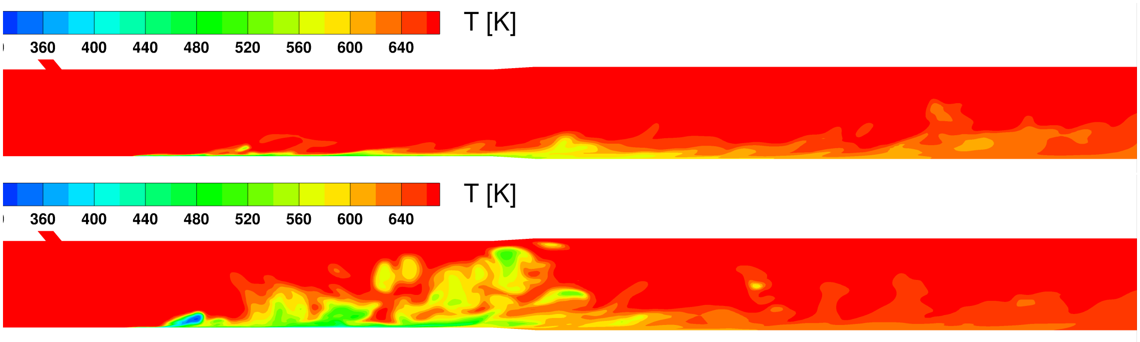

Figure 7. Comparison of temperature evolution at 550 ms after first SOI for case 1 (top) and case 2 (bottom)

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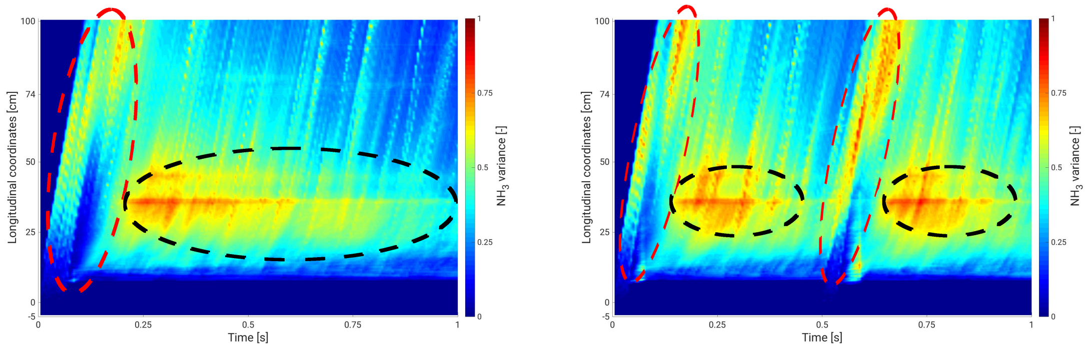

Figure 8. Comparison of NH_3 CoV evolution for case 1 (left) and case 2 (right)

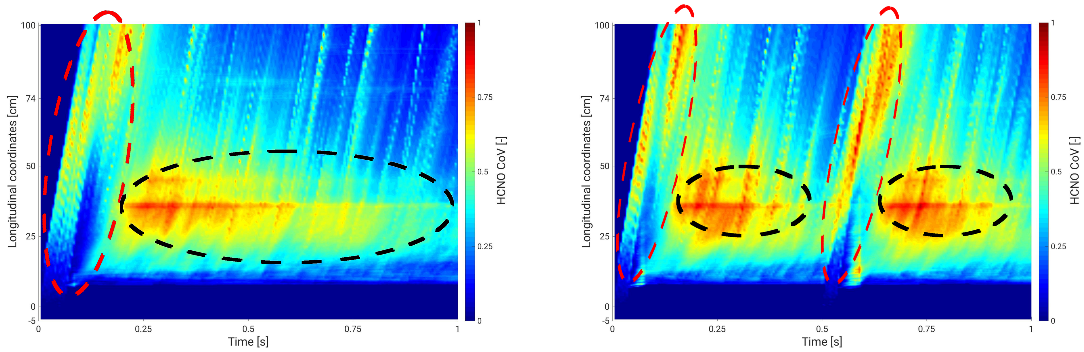

Figure 9. Comparison of HCNO CoV evolution for case 1 (left) and case 2 (right)

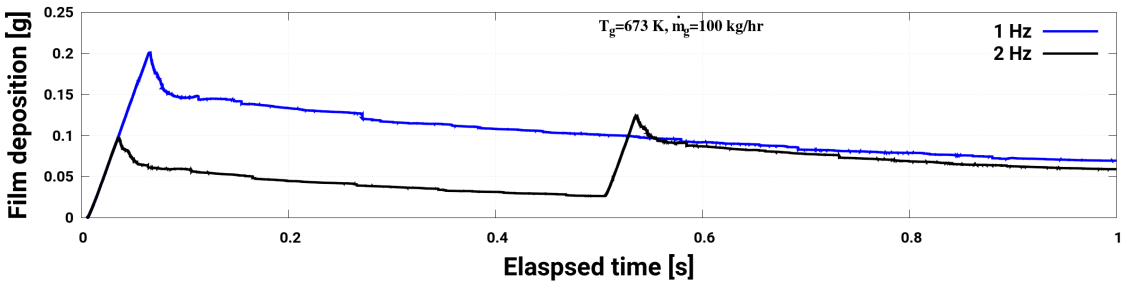

Figure 10. Comparison of adBlue deposition on SCR duct wall for case 1 (blue line) and case 2 (black line)