Numerical Simulations in Selective Catalytic Reduction Systems with an Emphasis on Injection Location

Martin Novák[1*], *Richard* Matas[2]

[1] Department of Power System Engineering, Faculty of Mechanical Engineering, University of West Bohemia, Univerzitní 2762/22, 301 00 Pilsen, Czech Republic
[2] Modelling and Simulations in Technical systems, New Technologies – Research Centre, University of West Bohemia, Univerzitní 2732/8, 301 00 Pilsen, Czech Republic

Abstract. This paper is a follow-up study to previous research conducted in the field of Selective Catalytic Reduction systems. The objective of this particular study is to identify a suitable injection location for urea water solution within a chosen geometry, matching the distribution commonly used in these systems. Numerical simulations using ANSYS Fluent software were conducted, utilizing an evaporation model that had been fine-tuned based on experimental data. The droplet size injected from the nozzle was also determined from experimental data. The boundary condition applied to the walls was the "Wall-Jet" model, chosen as a compromise for time efficiency. Over one hundred simulations were conducted at more than fifty locations, with the results presented here serving as interim findings. Future research will investigate the application of the recommended injection sites in geometries similar to those used in SCR systems.

1 Introduction

Selective catalytic reduction (SCR) is a technology used to reduce nitrogen oxide (NO_x) emissions from diesel engines, power plants, and other industrial processes. SCR involves injecting a liquid reductant, typically aqueous urea solution (also known as diesel exhaust fluid or DEF), into the exhaust stream. The reductant then reacts with the NO_x emissions over a catalyst bed, which converts the NO_x into harmless nitrogen (N_2) and water vapour (H_2O).

The SCR process is highly effective at reducing NO_x emissions, often by more than 90%. This technology is widely used in diesel engines, particularly in heavy-duty trucks and buses, to comply with emissions standards set by governments around the world. NOx refers to a group of air pollutants that are primarily composed of nitrogen oxide (NO) and nitrogen dioxide (NO_2). These gases are formed during high-temperature combustion processes, such as those found in engines, power plants, and industrial processes. NO_x emissions have a number of negative environmental and health impacts. They contribute to the formation of ground-level ozone, a major component of smog, which can have serious respiratory effects

* Corresponding author: novakm42@ntc.zcu.cz

on humans and animals. NO_x emissions also contribute to acid rain and can harm plant life, water quality, and ecosystems.

NO_x is primarily generated through high-temperature combustion processes, such as those found in engines, power plants, and industrial processes. Some common sources of NO_x emissions include:

- Transportation: Vehicles, including cars, trucks, buses and aircraft, are major sources of NO_x emissions. The combustion of fuel in vehicle engines generates high temperatures, which can lead to the formation of NO_x.
- Power Plants: Power plants that burn fossil fuels, such as coal, oil, and natural gas, also generate NO_x emissions. These plants produce electricity by heating water to create steam, which drives a turbine to generate electricity. The combustion of fossil fuels to heat the water can generate NO_x.
- Industrial Processes: NO_x can be generated by a wide range of industrial processes, such as those used in chemical manufacturing, metal processing, and cement production. These processes often involve high-temperature combustion, which can lead to the formation of NO_x.
- Residential and Commercial Heating: Some residential and commercial heating systems, such as those that burn oil or natural gas, can also generate NO_x emissions.

When DEF is injected into the exhaust stream of a diesel engine, it reacts with the NO_x emissions and breaks them down into harmless nitrogen and water vapour. This process occurs in the presence of a catalyst, typically made of metal oxides such as titanium dioxide or vanadium oxide, which facilitates the reaction.

The chemical reaction that occurs when DEF and NO_x combine is known as reduction. The urea in DEF breaks down into ammonia when it is heated in the exhaust system, and the ammonia then reacts with NO_x to form nitrogen and water.

The location of DEF injection is an important factor in the efficiency of the SCR system. The DEF is injected into the exhaust stream before it enters the SCR catalyst. The location of the injection point affects the mixing and distribution of the DEF in the exhaust stream, which in turn can affect the efficiency of the SCR system in reducing nitrogen oxide emissions.

The ideal injection location for the DEF is upstream of the SCR catalyst, where it can be well mixed with the exhaust gases. The injection point should also be located in a region of the exhaust stream that has a uniform temperature and flow rate, to ensure consistent mixing and reaction between the DEF and NO_x, but these requirements are not often met. If the injection point is too far upstream, the DEF may not have sufficient time to mix and react with the NO_x before it reaches the catalyst, reducing the efficiency of the SCR system. On the other hand, if the injection point is too close to the catalyst, the DEF may not be well distributed in the exhaust stream, resulting in an incomplete reaction and reduced efficiency. Overall, the location of DEF injection is an important parameter in the design and optimization of SCR systems, and must be carefully considered to ensure optimal performance and maximum reduction of NO_x emissions.

Despite the location of DEF injection being an important issue, there are not many articles which focus on this area. Jyothis et al. in [1] deal with simulations of urea-water solution (UWS), where they evaluate three different temperatures and velocities and compare their results with the study by Kim et al. [2]. Kim et al. [2] was used by Prabhu et al. in [3] to compare their UWS evaporation simulations with the experiment. These simulations included three different temperatures and angles in their study, which also included mesh sensitivity study. Two different velocities were evaluated by Khan et al. in [4] and their experiments were compared with simulations. Khan et al. obtained results with small differences. Their study was different because they included small inserts in their models where they evaluate deposits of an intermediate product which are created during decomposition of UWS. The influence of different temperatures was studied by Nayak et al. in [5] who compared their results with the experimental study by Wang et al. [6]. They concluded that their results are consistent with the experiments.

There are authors who deal with different conus angles of the injected UWS, such as [7] where Ye et al. looked at the influence of different flow velocities and droplet size. The influence of the spray angle, droplet size and injection velocity were investigated by Capetillo and Ibarra [8] who concluded that all of these three variables have a significant influence on the uniformity index of ammonia which is the main index used to evaluate their study.

Bayramoglu et al. [9] carried out simulations of a low-pressure system and a high-pressure system. Before they started, they tuned their calculations using an experiment by Sung et al. [10]. The authors in both articles used a mixing chamber and Sung used a static mixer to increase the efficiency of the SCR system. Sung carried out an experimental and CFD study of four different engine regimes and concluded that the best results were achieved by using the mixing chamber and a static mixer. Similar results were obtained by Maass et al. [11]. This study was experimental, supported by CFD simulations, where different types of nozzles were investigated. They introduced a static mixer to their design to calculate its influence, which was found to be positive, and they recommend using it. Lee et al. [12] state that it is important to deal with the location of injection, types of nozzles and, as previously mentioned, mixing. CFD simulations and an experimental study with mixers was done by [12]. Lee et al. concluded that their results were comparable and correct. One of their main results was that about 4.4% of the urea solution injected is converted into a wall film. By optimizing the injection load, (frequency), the nozzle angle, and the mixer configuration for optimal flow, the formation of the wall film can be reduced. This result shows that only a small amount of UWS is transferred to the wall film, so in our study we ignored it.

2 Investigated Case

This study builds on previous studies, specifically by Novák et al. in [13] and [14], thus it is their direct successor and uses the knowledge gained from them in further research. The model in this case is shown in Figure 1. The simulations are done in ANSYS Fluent 2021 R1. This version was used at the beginning of the whole research and for the sake of continuity it will be used until the end of it. The settings are the same as in the previous studies.

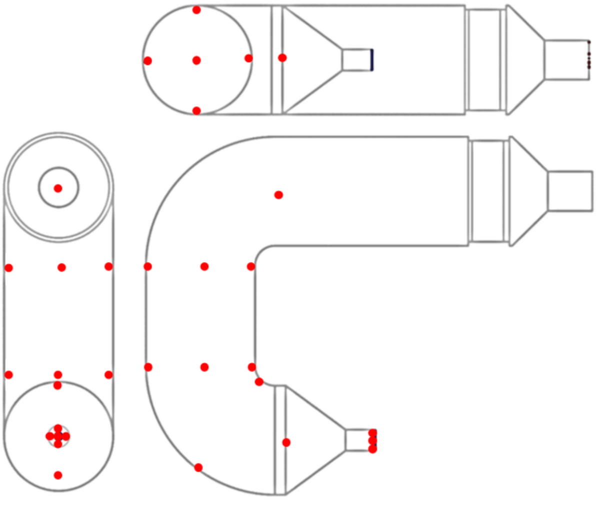

Fig. 1 Locations of injection in the investigated geometry

Two simulations were done for each different wall treatment, specifically the reflex boundary condition, to find out the differences between them, but the results were not significantly different. Therefore a wall-jet boundary condition was chosen because it is expected to be more accurate and closer to reality.

The wall-jet boundary condition can offer a variety of rebound directions and velocities for liquid droplets colliding with a wall. This boundary condition is appropriate for scenarios where droplets strike a heated wall without forming a liquid film, causing them to either adhere or bounce off the surface depending on their impact characteristics. The momentum flux resulting from the collision determines the direction and speed of the droplet particles. The momentum flux is a function of impingement angle ϕ and the Weber number. See Figure 2 [15] where H(ψ) is the empirical function for sheet height as a function of the angle and the drop leaves with the impingement ψ.

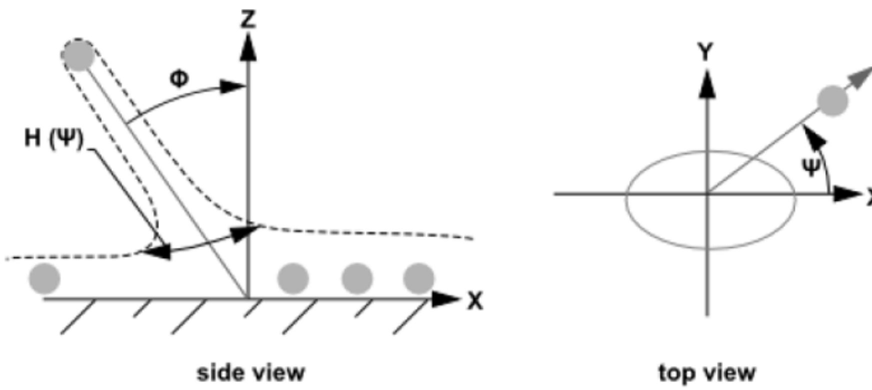

Fig. 2 Wall-jet boundary condition [15]

This boundary condition might not seem to be the right one, since it is possible to choose the wall-film version, but there are two approaches in ANSYS Fluent which can be used. One of them is Eulerian wall-film, which is very difficult to introduce to such a simulation because it is necessary to use small time steps, meaning the computational time would be too long for these sets of simulations. The second option is the Lagrangian wall-film which is recommended by the ANSYS Fluent User's Guide [15] for SCR catalyst, but there are a couple of restrictions. The most important in this case is that the wall-film must be less than 500 μm thick and the wall-film temperature must never exceed the boiling temperature of the liquid. The guide [15] recommends the wall-jet boundary condition in cases where the spray impacts a very hot wall, which is assumed in this case, since the operating temperature is constant and the SCR catalyst is usually located in closed spaces which are hot.

Ammonia is one of the emissions which is controlled because of ammonia slip, but droplets are not evaluated after the catalyst. It is assumed that all of the droplets which enter the catalyst evaporate on the small surfaces where there are low velocities and the catalyst has a high temperature which helps the evaporation process. In this model, a new boundary condition, "Porous Jump", is introduced at the inlet to the catalyst. This is sort of an upgrade to the boundary condition "Interior", the advantage here is that additional features may be set. In this particular case, the "Trap" option is selected which immediately evaporates all the remaining droplets. This means that no droplets enter the catalyst. Since it is not possible to simulate this process, the "Trap" condition is used here to get closer to reality.

The simulations include "only" the evaporation of UWS and not the conversion of urea to ammonia. Therefore, in this case, only the droplets are observed to evaporate, from which we can consider how well the system is designed. A well-designed system will ensure evaporation of the UWS before entering the catalyst itself without considering evaporation in the channels ("Trap" boundary condition here).

This study aims at finding the best possible location for the depicted geometry, which was chosen according to a commonly used geometrical exhaust duct for a SCR catalyst. Some improvements were made to the flow field, which was published in a previous study by Novák et al. [13]. In Figure 1 the red dots show the different UWS injection points. Dozens of simulations were performed in fundamentally different configurations. One set of calculations considered a uniform inlet profile, the other set considered a rotating inlet velocity profile. Further, each calculation had only one UWS injection point. Several different injection points were created from most of the points shown. In simplified terms, the injection was perpendicular to the pipe (1), the second direction was upstream at 45° (2), the third direction was downstream at 45° (3), and the other two were perpendicular to the previous two so that they were facing the "wall" (4a and 4b). A simplified diagram of this is shown in Figure 3.

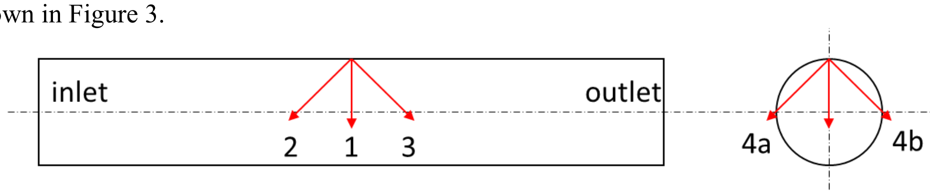

Fig. 3 Illustration of the injection direction logic

3 Evaluation

Figure 1 shows one of the basic setups of an SCR system. More than one hundred simulations were done in this particular case. It is impractical to show all the results, so only those with good results and those with the worst results will be listed here.
As mentioned above, the simulations of one particular injection point were done with two different cases. One of them had uniform inlet flow, which means that at the inlet there is the same velocity magnitude on the surface. The second case had a rotational velocity field at the inlet as mentioned in [13]. This approach was chosen because these are the limit states in which the device can operate. Therefore, the results from both of these simulations must meet the same conditions to be considered good. If the results from one type of calculation are not good enough, it means the variant is disqualified. Some cases were calculated with "Reflex" boundary condition on the walls instead of "Wall-Jet", but it had no major impact on the evaluation.

The evaluation is based on the uniformity index (UI) and area weighted concentration of droplets (DPM). Both of these values are evaluated before the catalyst bed. The results are not influenced by the "Porous-Jump" condition. There are other variables which are evaluated, but their results are not indicative of the quality of the individual variants. For example, evaluation of flow distribution, which is relevant for comparison of different geometrical modifications, is not applicable here because the geometry is the same in every simulated case and the injection location does not influence the stream, so the UI of flow is equivalent for all cases. The same evaluation logic is also applicable for pressure losses etc.

The uniformity index was described in a previous article [13]. The same evaluation is used here but the variable is different in this case, particularly as it is a mean mass fraction of the gaseous component of urea. Evaporated urea is an important intermediate step in the chemical reaction necessary for creating ammonia. As described by Payri et al. in [16], the chemical process follows these two steps according to equations (1) and (2).

$$(NH_2)_2CO \rightarrow NH_3 + HNCO \quad (1)$$

$$HNCO + H_2O \rightarrow NH_3 + CO_2 \quad (2)$$

The first equation (1) shows thermolysis caused by the high exhaust temperature, the second equation (2) is hydrolytic, where isocyanic acid transforms to ammonia in the presence of water vapour. Since the chemical reactions are not included in the presented simulations, the distribution of urea is used for evaluation. The UI of the mean mass fraction of the selected variants are shown in Figure 5. The injection location of the selected variants is shown in Figure 4. The variants shown in Figure 4 are specifically chosen to illustrate good and bad results.

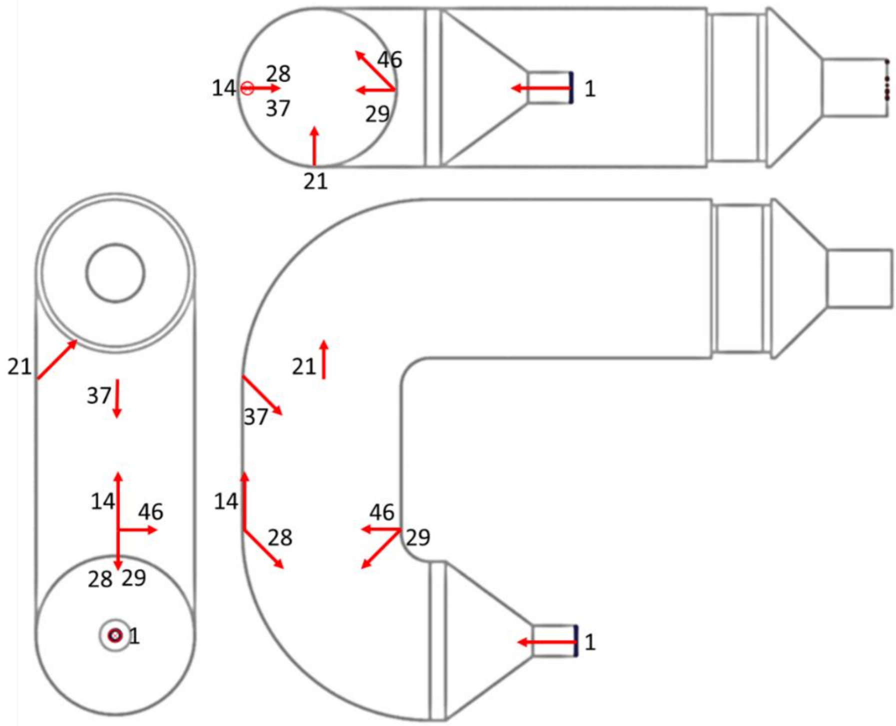

Fig. 4 Injection locations and directions of a selection of good and bad variants

Figure 5 contains results from selected variants, the displayed variable is the mass-weighted average of DPM concentration [kg/m^3]. It describes the number of droplets which are not evaporated immediately before they enter the catalyst bed, because the "Porous Jump" is set on the inlet to the catalyst, meaning all of the droplets are evaporated. But for evaluation it is important to know the state right before it happens. Variants 1 to 15 are always calculated in three cases, once with "Reflex", once with "Wall-jet" and once with "Wall-jet" and the uniform inlet. The following variants, 16 to 51, are always calculated with "Wall-jet", so there are only two cases of calculation. It is assumed that all of the calculated cases for one injection location have to meet the same criteria (none of them could have much greater values). The best variant would be the one where all of the calculated cases would evaporate all the droplets before the catalyst bed, but this seems to be an impossible task in reality. Aiming for complete evaporation is too high a goal, but it is possible to decide which locations are better than others for injecting the UWS. In Figure 5 the lower values are the desired ones.

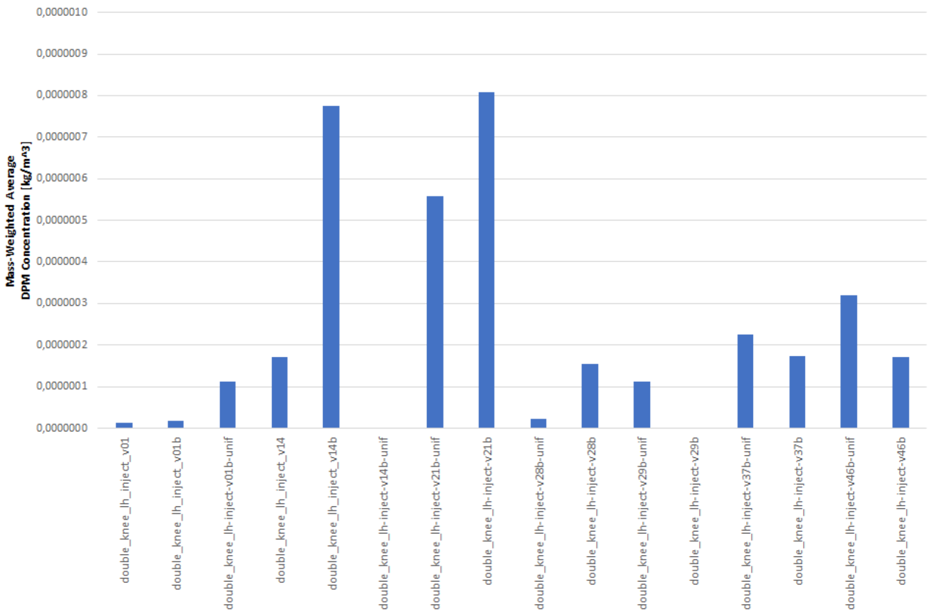

Fig. 5 Mass-Weighted Average of DPM Concentration

It is obvious from Figure 5 that variants 1, 28 and 29 have the lowest values and might be considered as good variants. The rest of the depicted variants have higher concentration numbers. Where to put the line of suitable and unsuitable variants is ambiguous but, from a broader point of view (all of the calculated variants), a value below 0.00000025 $[\mathrm{kg/m^3}]$ seems reasonable. With a more rigorous approach, a significant number of options would drop out that have very good potential. The previously mentioned number meets 19 variants, only nine variants would pass the stricter condition 0.0000001 $[\mathrm{kg/m^3}]$, but this is not the only indicator, so the higher value is considered. The selected variants with a more restrictive condition would not correspond to the attempt to describe the recommended injection locations in a more general way, which is the aim of this work.

The uniformity index of the mass-weighted mean mass fraction of $CO(NH_2)_2$ values of the chosen variants are displayed in Figure 6. It was mentioned in [13] that values over 0.94 $[-]$ are considered as good results, but some authors aim at even higher numbers such as 0.98 $[-]$. [17] In this study most of the variants meet the lower requirement in order to not disqualify too many variants. Therefore it is necessary to use a higher value, closer to that recommended by Lu et al. in their study, so 0.97 is chosen. In Figure 6 it is desirable to have high numbers, which is the opposite of the previous one. Variants 1, 21, 29 and 46 meet the desired requirement. This value describes the uniformity of the evaporated urea before it enters the catalyst. The rest of the displayed variants reach high values (except for variant 14) of UI.

According to the results displayed here, variants 1 and 29 are the ones that should be recommended for installation in an SCR system. But from a practical point of view, variant 1 is difficult to install since it is in the middle of the duct, thus only variant 29 is reasonable and meets the required constrains.

The best variants are displayed in Figure 7. There are twelve variants which meet both criteria mentioned above. Variants 1 and 5 are not recommended for obvious reasons. It is very difficult to install the nozzle right behind the turbocharger in the middle of the channel. These are the results that fit perfectly to the chosen geometry. It is not easy to make general recommendations from these conclusions, so it is necessary to also look at the rest of the results.

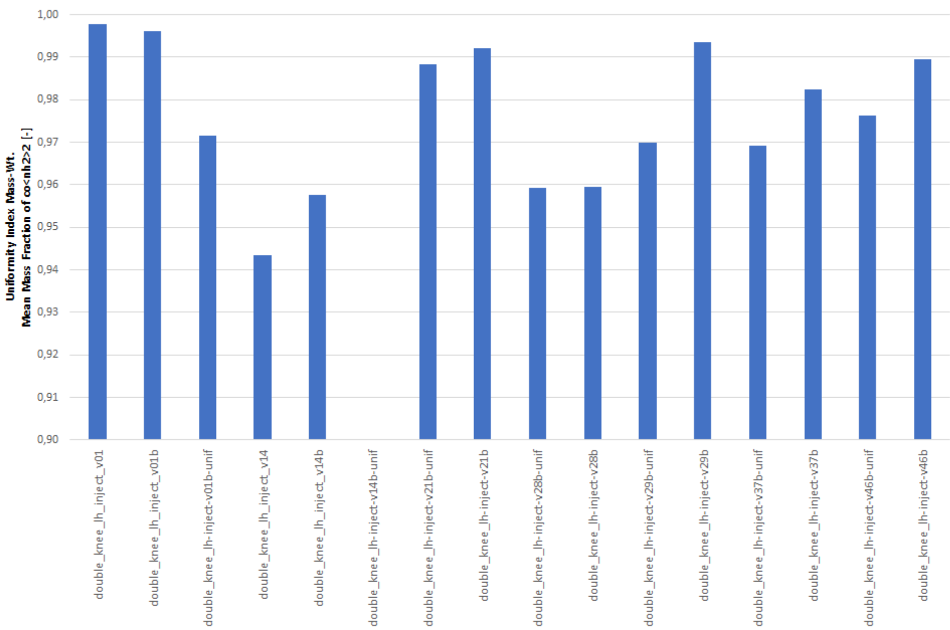

Fig. 6 Uniformity index mass-weighted mean mass fraction of evaporated urea

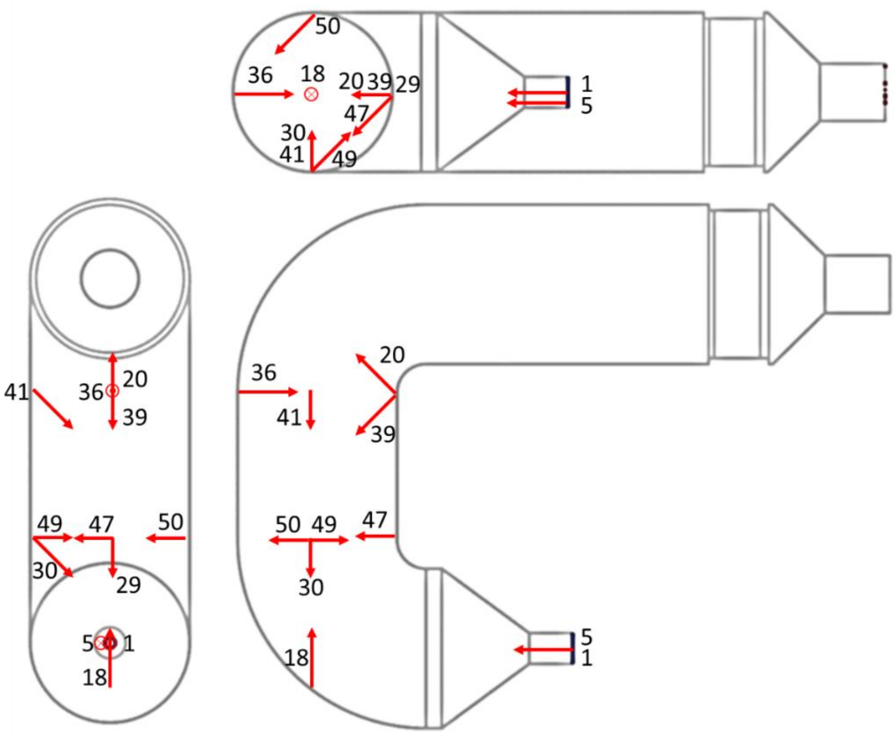

Fig. 7 Injection location and direction of the best variants

4 Conclusion

Considering all the relevant results, which include those that do not reach the required maximum values of the criteria but are very close to them, the following conclusions can be drawn. It is generally recommended to choose locations at the elbows where the vortices are expected to increase the residence time of the particles, thus prolonging the residence time in the channel and thus evaporating most of the droplets. It is also recommended to inject the liquid downstream, upstream or perpendicular to the channel and not towards the walls near the injection location.

Further research will focus on the application of a Lagrangian wall-film, since using the Eulerian approach to wall-film is unrealistic in this case, due to the small time step required. Furthermore, the general results obtained by this research will be applied to other geometries that have already been shown in the previous paper. The last part of the research will be the application of the chemical equations, tuning the calculation according to the experiments and applying it to selected variations.

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