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Numerical Simulations of Droplet Evaporation in a SCR System Submodel with Hot Air Flow

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Abstract. This paper focuses on the numerical simulation of liquid droplet evaporation in a hot air flow in a submodel which is created in conformity with a real life application in a Selective Catalytic Reduction (SCR) system. Simulations of droplet evaporation processes in the SCR system are complex, so it was necessary to create a submodel to verify the stability of the evaporation model in ANSYS Fluent CFD code. Evaporation is a complex process which happens even below the evaporation point, but once the temperature of the liquid reaches this point the process becomes a lot faster. Simulations are made with AdBlue® which is a liquid made of urine and water. The simulation results are compared with available experiments and show that the applied method for droplet evaporation is suitable. These successful results mean that the next step is the application of this model to a complete SCR system.

INTRODUCTION TO SCR SYSTEMS

Selective Catalytic Reduction (SCR) is a process used in combustion engines to reduce emissions according to European emission standards. There are other technologies used in cars to reduce the amount of particulate matter (PM) but they also increase the amount of NO_x in the flue gas [7]. But SCR is not applied only in a vehicle engines – it is also applied in stationary applications such as coal or gas power plants where the reduction of NO_x is even more important because these plants generate a huge amount of emissions [3]. Reduction of NO_x is achieved by injecting a fluid made of urea (32.5 % of mass) and water (67.5 % of mass) called AdBlue® into the flue gas. AdBlue® should evaporate as fast as possible because the gaseous state of this substance (mainly ammonia) participates in the chemical reduction which occurs on the catalyst.

Temperatures during these chemical reductions are in the interval 573–673 K. There are three basic chemical equations, which are shown in (1).

$$\begin{aligned} 4NO + 4NH_3 + O_2 &\rightarrow 4N_2 + 6H_2O \\ 2NO_2 + 4NH_3 + O_2 &\rightarrow 3N_2 + 6H_2O \\ NO + NO_2 + 2NH_3 + O_2 &\rightarrow 2N_2 + 6H_2O \end{aligned} \tag{1}$$

From these equations it is obvious that ammonia is a crucial part of the reduction. There are several secondary reactions and it is also possible that urea reaction occurs in the catalyst, but these are not important for the purposes of this paper.

The most important part for the reduction is the ammonia which causes the chemical reaction [5]. It is important to evaporate AdBlue® as fast as possible after injection and mix it into the whole stream of the flue gas so it is properly distributed on the catalyst surfaces [4].

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The basic scheme of the SCR system is shown in Fig. 1. It is a complex part of an exhaust system which consists of many different parts to reduce emissions. This paper is focused only on a small part of this device, which is the evaporation of the AdBlue® droplets. It looks like an unimportant problem from a global perspective, but for the catalyst reactions to work correctly it is a crucial part of the whole process.

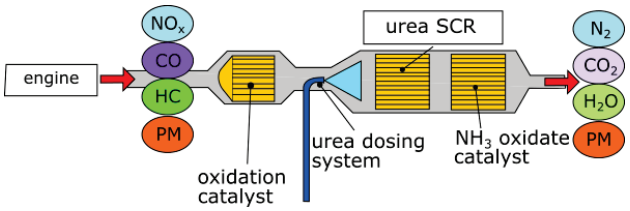


FIGURE 1. Basic SCR scheme [7]

Since the velocities in the exhaust duct are high and the droplet dwell time in the pipeline is small it is impossible to model the evaporation before the droplets enter the catalyst, so it is difficult to evaluate whether the software does the computation correctly and the evaporation process is valid [2, 6]. For validation purposes, it is important to use an easier geometry to ensure the quality of the ANSYS Fluent model.

CFD MODEL

As mentioned above, it is important to evaluate the proper functioning of ANSYS Fluent, which is the software used to simulate the evaporation process. The Discrete Phase Model (DPM) allows simulation of a discrete second phase in a Lagrangian frame of reference and the evaporating droplets are modelled in this way. The evaluation of this is the main topic of this paper. Experimental study of this phenomenon is difficult to observe, especially in the fluid stream inside the channel, so the experiments are mostly done on easier examples, such as single droplet evaporation in a heated chamber. This droplet is hanging on a thin string and the surrounding air is heated and exchanged, but the velocity of the air which flows around the droplet is negligible and it is included only because the droplet evaporates and saturates the surrounding air, so it has to be exchanged and the evaporation process may continue. This experiment was performed by Wang [1] and his results are discussed and compared with the simulations later.

The model in our verification case was simplified to a simple tube which is shown in Fig. 2. The tube has a circular cross section. The pink cone on the right side of the Fig. 2 shows the position of the injection of the droplets. The tube diameter is 0.264 m and its length changes from 10 to 80 m as a function of droplet diameter. The mesh size is from 8 million to 64 million cells. The inlet flow speed is set to 1 m/s and the temperature of the inlet flow is set to 573 K, which is the lowest recommended temperature for the reduction process.

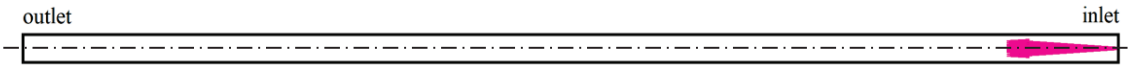


FIGURE 2. Geometry of the CFD model

The simulations are done with the energy equation. Species transport is included because there is a transition of liquid urea and water to a gaseous state. The droplets of AdBlue® are multicomponent, consisting of 32.5 % urea and 67.5 % water. The Reynolds number according to equation (2) is low, which indicates that the flow should be laminar. The simulations are also done with a turbulent model because in a real life case the flow type is not only determined by the local Reynolds number. The SST k-ω model was chosen because it is planned to use it in simulations of real devices. Droplets always have only one diameter size in each model – 40, 100, 200, 300, 500, or 920 μm.

$$\mathrm{Re} = \frac{wd}{\nu} \tag{2}$$

RESULTS OF THE SIMULATIONS

More than twenty different simulations were done to obtain satisfactory results which could be compared with experimental studies. Initial simulations were done with pure water without urea, but the results were incomparable to the experiments done with AdBlue®, so the results from water evaporation simulations are not presented here.

Once the model was prepared it was necessary to decide which diameter of the injected droplets were to be used. The diameter is chosen according to the available results from an experiment with nozzles manufactured by Lechler GmbH and also one size according to the experimental study by Wang [1]. The proper setting of the simulation is also important because there are many possibilities for simulating the flow and the droplets. Both steady and unsteady tracking of the particles is available and both of these approaches are applied in these simulations to compare their results. Since the flow should be laminar, laminar equations are also used, as well as the SST k-ω turbulent model even though the Reynolds number is low.

The best way to display the droplet evaporation is on a graph where the x-axis shows the time t divided by the initial square diameter of the droplet d_i^2. This gives comparable results and readable values. The y-axis shows the current square diameter d^2 divided by the initial square diameter of the droplet d_i^2 , so it is a dimensionless variable which shows the loss of mass during the evaporation process.

The result of the first simulation is shown in Fig. 3 a). The viscous model is laminar and particles are tracked steadily. The velocity of the flow and injected particles are the same, so the heat exchange is lower than in the second case shown in Fig. 3 b), where the velocity of injected particles is 17 m/s which is much higher than the velocity of the flow. These particles are small, so after a short period of time in case b) in Fig. 3 the velocities match the flow speed. These results in both cases are non-physical because the diameter of the droplets jumps from the current value to zero without disappearing from the flow (so they do not evaporate, they just change their dimensions), and after some unpredictable time they appear again with an irrelevant diameter.

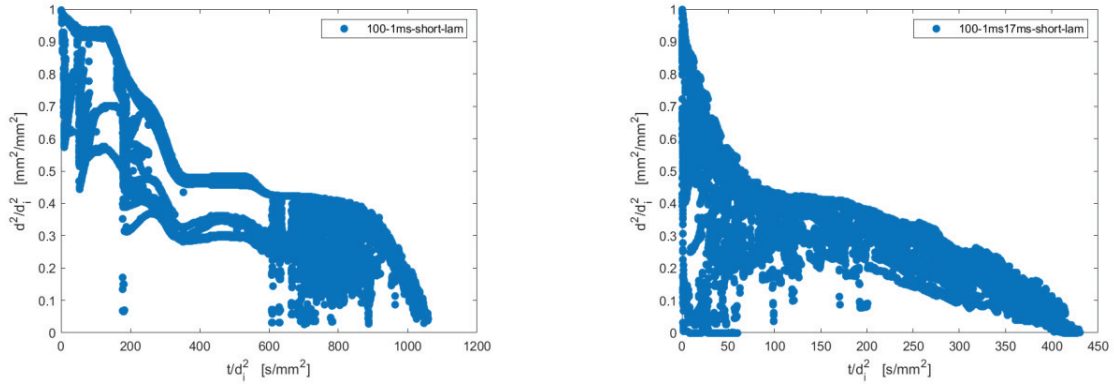


FIGURE 3. The results from simulation of laminar flow and the size of the droplet 100 μm, a) the velocity of the injected droplet 1 m/s, b) the velocity of the injected droplet 17 m/s

The second pair of results is shown in Fig. 4. On the left side a) are droplets with diameter 200 μm and the speed of the particles in the inlet is the same as the velocity of the stream. The behaviour is still non-physical as in the previous pair of results, but the results approach the experimental results. It was found that the non-physical behaviour is independent of the size of the droplets. So the laminar equations for solving the flow are inappropriate, and even though the Reynolds number is low, the turbulent model has to be used. Since it is a simple tube, the turbulent model k-ε was used to stabilize the result which is expected to model the flow close to the walls better than the k-ω. But as is shown in Fig. 4 b), the results are still incorrect.

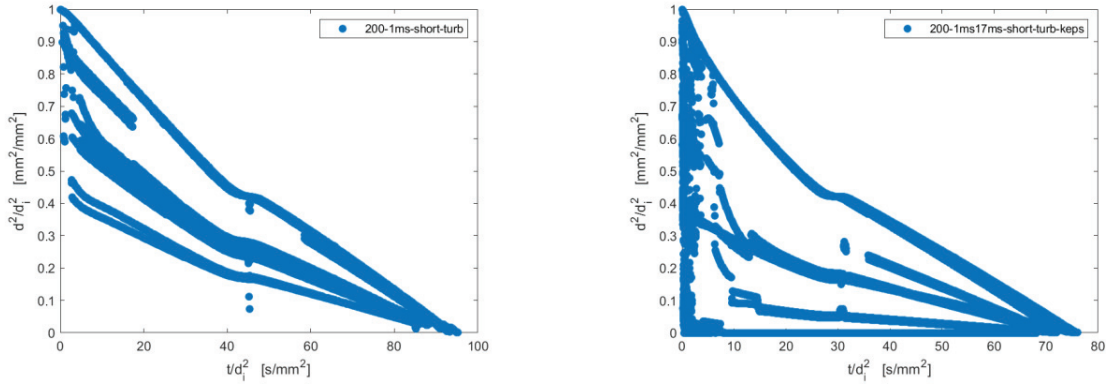


FIGURE 4. a) the results from simulation of turbulent SST k-ω model, the size of the droplet 200 μm, and the velocity of the injected droplet 1 m/s, b) the results from simulation of turbulent k-ε model, the size of the droplet 200 μm, and the velocity of the injected droplet 17 m/s

The simulations have been done with steady particle tracking until now, and the results are still incorrect. So the problem has to be approached with unsteady particle tracking which is, according to the numerical essence of the modelling, physically correct. Figures 5 and 6 show the results of four different sizes of droplets. All of the simulations are done with the SST k-ω model. The different velocities of the stream and the injected particles (the results are the same even though the velocity at the inlet is the same) and the particles are tracked unsteadily. Simulations with this setup are stable and correspond to the experimental study done by Wang [1].

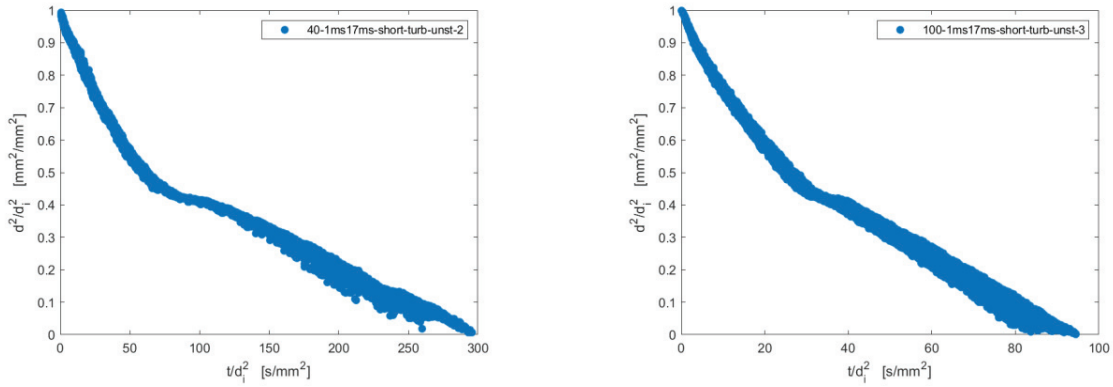
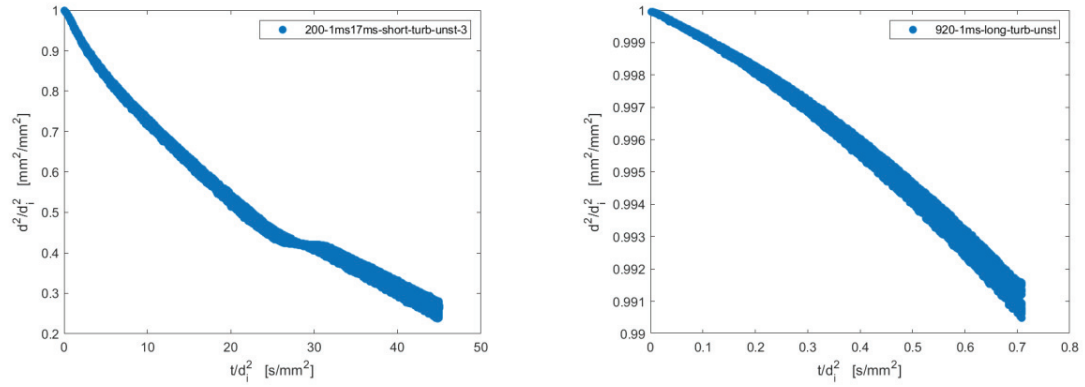


FIGURE 5. a) the results from simulation of turbulent SST k-ω model, the size of the droplet 40 μm, and the velocity of the injected droplet 17 m/s, b) results from simulation of turbulent SST k-ω model, the size of the droplet 100 μm, and the velocity of the injected droplet 17 m/s

Figure 6 shows a pair of results with droplets diameter a) 200 μm and b) 920 μm. Both of these simulations are unfinished because the simulation is time consuming and they are done just to prove that the simulation setup is valid even for bigger droplets. This assumption is correct, even though these two simulations are incomplete. The variant with the bigger size of droplets is calculated because this diameter was placed in Wang's [1] experiment but it is not possible to process the simulation since the evaporation time is too long and the simulation would require a huge amount of computational time.

The results from the simulations are comparable with the experiment, so it is possible to assume that ANSYS Fluent is a satisfactory tool for simulating the evaporation process of the droplets in a free stream. From the results it is possible to see that the bigger the initial diameter, the smaller the ratio between evaporation time t and the initial square diameter of the droplet d_i^2.

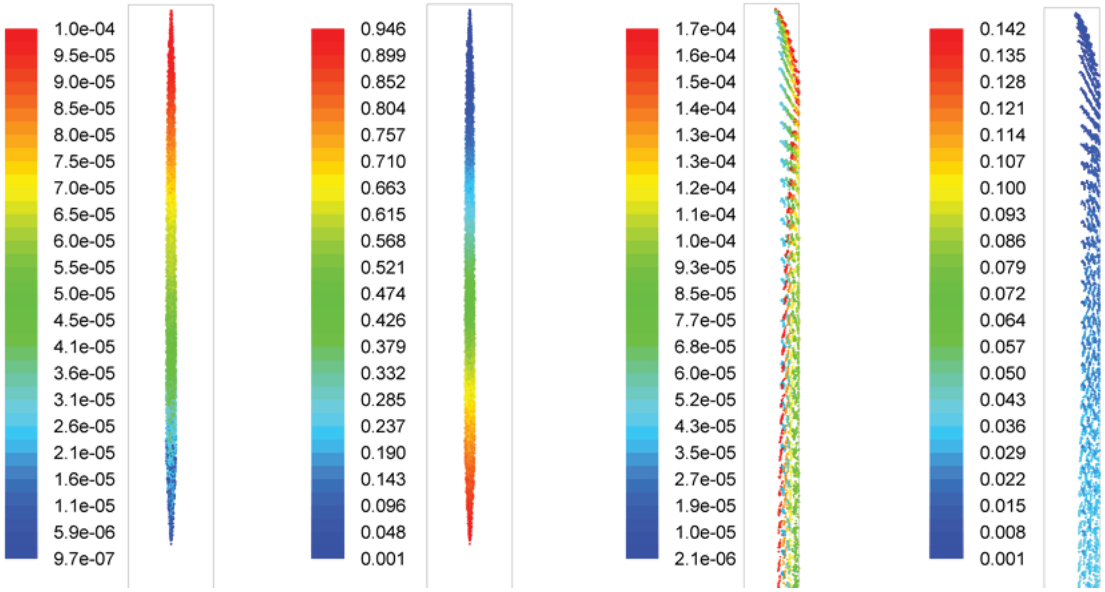
The results from other simulations show that the different speed between the droplets and the flow helps to augment the evaporation process because the heat transfer coefficient increases, which has a positive effect on the heat transfer from the flow to the droplets.



a) b)

FIGURE 6. a) the results from simulation of turbulent SST k-ω model, the size of the droplet 200 μm, and velocity of the injected droplet 17 m/s, b) the results from simulation of turbulent SST k-ω model, the size of the droplet 920 μm, and the velocity of the injected droplet 1 m/s

The evaporation process is shown in Fig. 7. Figure 7 a) shows the droplets diameter [m]. The particles are coloured according to their dwell time [s] in the channel in Fig. 7 b). The biggest droplets are at the inlet and the time is basically zero. At the end of the evaporation process, the time is maximum because the dwell time of the particles is just before their diameter becomes too small and they become completely evaporated. The droplets are injected into the free stream, which is turbulent most of the time and there are vortices, wakes, etc.



a) b) c) d)

FIGURE 7. Evaporation process of droplet with initial diameter 100 μm, a) particle time [s], b) particle diameter [m] and results of evaporation process in wall film, c) particle diameter [m], d) particle time [s]

It is impossible to ensure that all of the injected droplets are evaporated in a free stream. The droplets might adhere to the walls and create a wall film. Since the walls are also heated by the flow, the fluid from the wall film is also evaporated. This wall film occurs in most cases, so it has to be included in the simulations and should be

verified. It is still impossible to simulate the evaporation of AdBlue® with the wall film at the moment, but simulation with water as the material of the droplets is possible. The results from simulation with water droplets and wall film are shown in Fig. 7. Gravity is included in this simulation. The direction of this force is perpendicular to the channel. The walls have a constant temperature and it is obvious that droplets in the wall film are quickly evaporated. Some of these droplets are reflected and go on through the pipe and their evaporation process continues. Figures 7 c) and d) display the particles injected into the channel in a direction which ensures that the droplets interact with the wall and allow the creation of the wall film. In Fig. 7 c) the variable is particle diameter [m] and in Fig. 7 d) the scale is a function of time [s].

COMPARISONS OF EXPERIMENT AND SIMULATIONS

Figure 8 shows the results from the experiment by Wang [1] and the presented simulations. The curve of the experiment shows an evident change in curvature which is caused by the different main component of the droplet. This effect is observed even in the simulation. The droplet diameter in the experiment is 920 μm. These big droplets are impossible to evaporate in a tunnel, so the experiment was done on a steady droplet. The simulations were not done in a similar manner because the application in real life devices requires evaporation in a channel. The real life applications are limited by the dwell time of the droplets in the duct. The simulations are therefore done in a simple pipe to achieve the closest conformity to a real life application. The experiments might seem to be different, but the results show similar behaviour even though the droplet size is different.

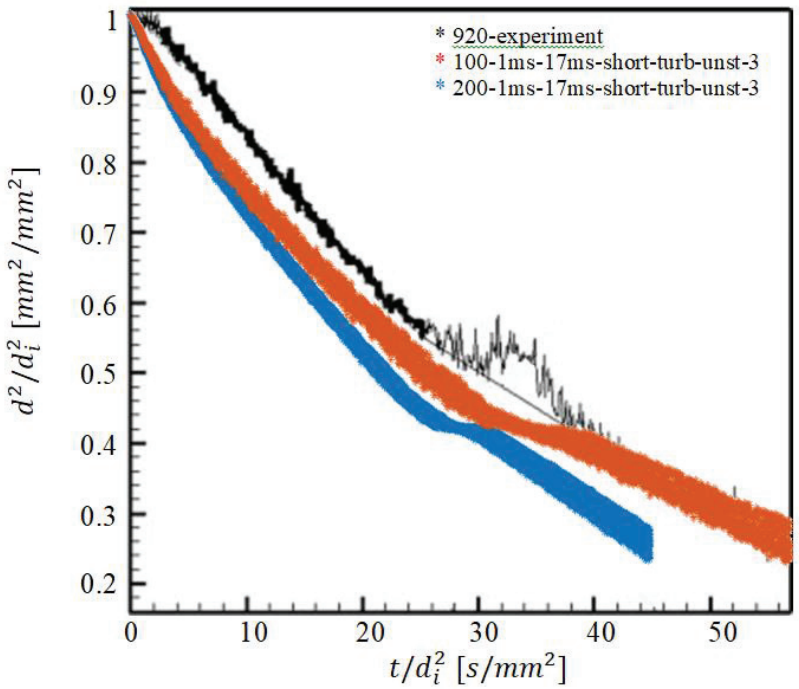


FIGURE 8. Results of experimental evaporation where temperature is set to 573 [K]. The initial droplets with diameter of 920 μm are shown in black [1], simulation with 100 μm are red and 200 μm are blue

CONCLUSION

The purpose of this study is to show the possibilities of evaporation simulations and the application of evaporation models in a free stream of hot air in the software. The numerical simulation of droplet evaporation was studied in the work. The CFD system ANSYS Fluent was used for a series of testing simulations of laminar and turbulent flows with evaporating droplets. The use of the models in CFD codes for evaporation had not been

verified for everyday use, so it was necessary to prove their correctness. Simulating a real technical problem is relatively complicated, so a simple submodel of a tube with a simple droplet injection was created.

The results from the simulations are not directly comparable with the experiments because the sizes of the droplets are different from the droplets in the experimental studies (and also in the application), but their behaviour seems to be the same. It can be concluded that it is possible to trust the simulations, and these models in the ANSYS Fluent system could be applied to a real SCR system. The flow must be considered as turbulent and the particles as unsteady for relevant results. The evaporation in the gas flow works correctly for single- and multi-component droplets but the evaporation on the wall works only for single-component droplets. This limitation will be further studied. The application to real geometry and conditions will follow.

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REFERENCES

1. T. J. Wang, S. W. Baek, S. Y. Lee, D. H. Kang and G. K. Yeo, "Experimental investigation on evaporation of urea-water-solution droplet for SCR applications", *AIChE J.,* 55: 3267-3276. doi:10.1002/aic.11939, (2009).
2. D. T. Ryddner & M. F. Trujillo, *Emiss. Control Sci. Technol.* (2015) 1: 80. https://doi.org/10.1007/s40825-014-0006-3
3. D. Cobb, L. Glatch, J. Ruud and S. Snyder, "Application of selective catalytic reduction (SCR) technology for NOx reduction from refinery combustion sources", *Environ. Prog.,* 10: 49-59. doi:10.1002/ep.670100116, (1991).
4. Y. Xiao, X. Tian, P. Zhou and W. Zhang, "Study on evaporation and decomposition process of urea water solution in selective catalytic reduction system", *Materials Research Innovations,* 18:sup2, S2-908-S2-913, DOI: 10.1179/1432891714Z.000000000533, (2014).
5. M. Stein, V. Bykov and U. Maas, *Emiss. Control Sci. Technol*. (2017) 3: 263. https://doi.org/10.1007/s40825-017-0075-1
6. K. Nishad, A. Sadiki and J. Janicka, "Numerical Investigation of AdBlue Droplet Evaporation and Thermal Decomposition in the Context of NOx-SCR Using a Multi-Component Evaporation Model", *Energies.* 11. 222. 10.3390/en11010222, (2018).
7. Selective Catalytic Reduction. IndiaMART [online]. Delhi: IndiaMART InterMESH [cit. 2019-04-17]. Available at: https://www.indiamart.com/proddetail/selective-catalytic-reduction-10683297197.html