THERMAL TRANSFER BETWEEN COMBUSTION GASES OF M.A.C. AND THE DROPS OF ADBLUE LIQUID

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Abstract: *In this paper is studied heat transfer, trajectory and evaporation time that occurs in the case of a drop of AdBlue that is injected into a gas flow at temperatures above 700K. The case of two configurations for piping where the vaporization process takes place was considered. We aim to analyze the trajectory of the Adblue particle in the catalyst channel, the partial pressures of the vapors formed in the piping, the mass fractions of the liquid mixture and the evolution of the mass concentration. This analysis highlights how a drop of substance evolves in the flue gas duct in compression-ignition engines (M.A.C.) using selective catalytic systems (SCRs) taking into account the chemical processes that help increase depollution.*

Keywords: *heat transfer, evaporation, droplet, AdBlue.*

1. Introduction

Due to the fact that NOx emissions (nitrogen oxides) becomes a global concern lately in M.A.C. it is necessary to study methods of improving them.

One constructive element that has been developed in solving depollution problems is SCR (Selective Catalytic Reduction). Selective Catalytic Reduction (SCR) is an effective technology for controlling NOx emissions from diesel car engines. For this, a reducing agent (usually ammonia, NH3) is introduced upstream of the SCR catalyst. In automotive applications Fig. 1, a solution of water and urea (AdBlue) is often used to produce ammonia.

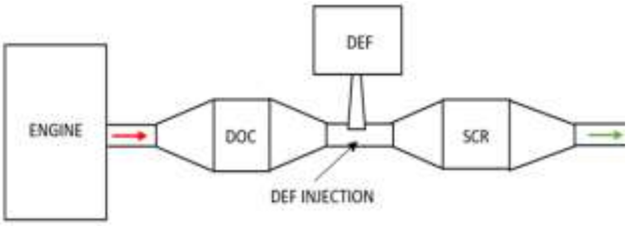


Figure 1: *Scheme of a selective catalytic reduction system (SCR).*

This system involves a chain of chemical reactors located at key points that perform chemical conversions to generate non-toxic elements (nitrogen and water). A basic schematic is illustrated in Fig. 1 wave, DOC - Diesel Oxidation Catalysts, DEF - Diesel Emissions Fluid.

The chemical reactions that take place are due to the system passing through several phases. In other words, chemical reactions take place between the liquid and a gaseous environment at high temperatures (exhaust gas).

The problem we study highlights the thermal exchange when injecting a substance particle into a gaseous environment at a certain pressure and flow rate, in which the dispersion and vaporization process of the substance droplets takes place.

In practice and in the specialty literature it is highlighted that chemical reactions take place at temperatures above 700 *K*. Cold starting and operating mode at relangations do not have the ability to provide a suitable temperature for the chemical process inside the SCR catalyst and this is partial decomposition of AdBlue. To solve this inconvenient, it is necessary to study how particle vaporization, trajectory and mass dispersion. We aim to simulate the evaporation process of a pure AdBlue drop to understand how to propagate the dispersion phenomenon and the trajectory in two predefined configurations.

2. The convective thermal exchange at AdBlue injection into a hot gaseous flow

We have developed a simulation model for a single spherical droplet of pure substance that is injected from a conical nozzle into a gaseous environment considered continuous by assumption. The evolution of the droplet is studied to determine the different states it goes through. The vaporisation phase, pressure evolution, mass fraction of the substance and liquid particle trajectory are analysed.

Thermodynamic phases are governed by continuity equations, moment, phase and temperature transport [1-7].

A drop is considered to have an initial T_l temperature at the time of injection by the conical nozzle in a gaseous stream with an initial T_g temperature and the density ρ_g. For practical reasons by experimental determinations, the drops can be considered as spherical drops of 10-100 μm. For the calculations, the model was adopted by Brin A. in [7].

The motion of a single liquid droplet in a gaseous environment is described by a differential equation of the form:

$$\frac{dv_x}{dt} = \frac{3C\rho_g v_x}{8\rho_l R_l} v_{tub}, \tag{1}$$

$$\frac{dv_z}{dt} = \frac{\rho_g - \rho_l}{\rho_l} g - \frac{3C\rho_g (v_z - u_g)}{8\rho_l R_l} v_{tub}, \tag{2}$$

$$\frac{dx}{dt} = v_x, \frac{dz}{dt} = v_z, \tag{3}$$

where v - the drop speed of AdBlue, t - Time, C - coefficient of aerody-namic resistance of air, ρ_l - density of AdBlue, R – radius of doplet.

For the law of conservation of mass we obtain the equation for changing the R_l radius of the substance drop:

$$\frac{dr_l}{dt} = \frac{\gamma(\mathrm{Re})(\rho - \rho_s(T_l))}{\rho_l} \tag{5}$$

where: ρ - vapour density of ammonia-water solution (AdBlue) in the gas stream [10], γ - mass transfer coefficient, Re - Reynolds number.

From the law of conservation of energy follows the equation of variation of the droplet with time:

$$\begin{aligned}\frac{dT_l}{dt} &= \frac{3[\alpha(\mathrm{Re})(T_s - T_l)}{C_l \rho_l R_l} - \\ &- \frac{3[\gamma(\mathrm{Re})(c_w T_l - U)(\rho - \rho_s(T_l))]}{C_l \rho_l R_l} + \\ &+ \frac{3[\varepsilon(T_g^4 - T_l^4)]}{C_l \rho_l R_l}\end{aligned} \tag{6}$$

where: U - latent heat of phase transition per water molecule, ε - absorptivity, α - heat transfer coefficients, σ - Stefan-Boltzmann constant.

In Eq. (6) is taken into account between the convective flow in the droplet, evaporation phenomenon in the hot combustion gas flow and the radiative phenomenon associated with heat transfer. We found that there is a direct connection between the terms related to evaporation of substance molecules and convective heat transfer [6,7]. In Fig. 2 the variation of the AdBlue droplet diameter with time has been plotted.

Initial conditions were taken for a stream of hot gas flowing through the injected droplets of AdBlue at temperature at T_g=*700K* and velocity u_g=10 *m/s*, for an initial droplet velocity uc = u_c = 0.1 *m/s*, at initial droplet temperature T_i = 293 *K*. A vapour density of AdBlue in the gas stream was taken as ρ = 1087 kg/m^3. In the approximation of a continuous flow, the rate of droplet change, depends on the mass transfer coefficient γ and the Reynolds number *Re* [6, 7] at the initial time of entry of a droplet into a flow. If the diffusion phenomenon is considered, the rate of change of droplet size is directly proportional to time, as shown in Fig. 2.

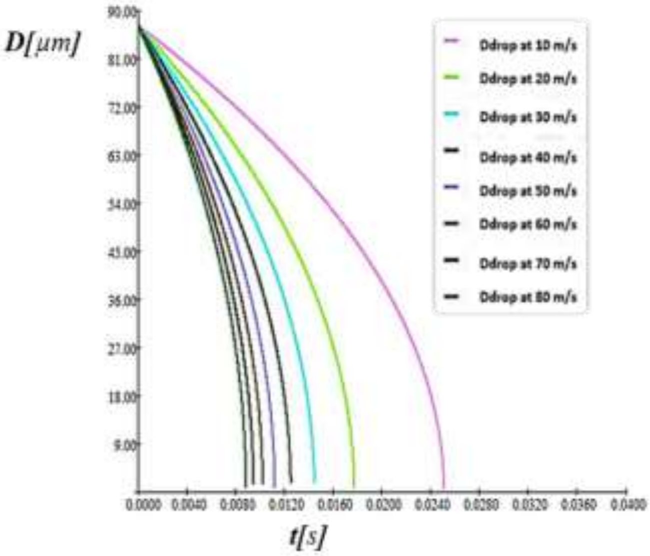


Figure 2: *Variation of droplet diameter D during vaporization at T=700K.*

2.2 Boundary condition

Fig. 3 is a schema of the processes that take place when phases change. Thus as illustrated, the liquid droplet, due to the turbulent gas flow, will be dispersed in the tubing as it partially vaporizes and mixes with the hot gases.

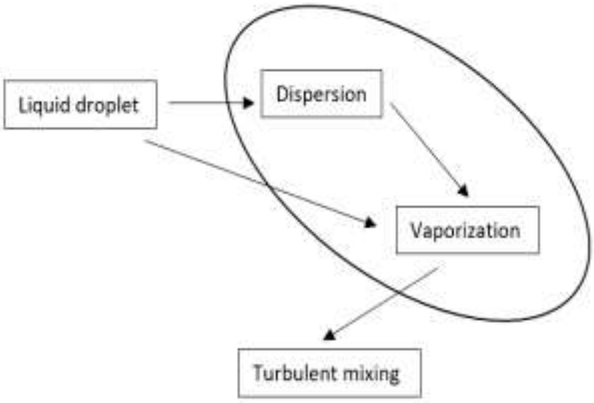
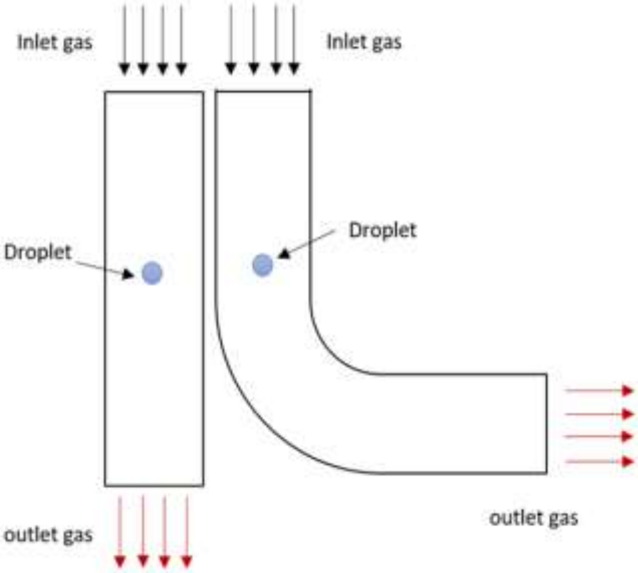


Figure 3: *Schema of the AdBlue droplet vaporisation process in a hot gaseous environment.*

To simulate the process, two different configurations have been considered to study the vaporization process of a liquid droplet in a hot air flow. The first configuration consists of a straight pipe (Fig. 4a), and the second configuration consists of a pipe oriented at 90° Fig. 4b).



a) b)

Figure 4: *Pipeline configurations for the study of droplet vaporization evolution in a gaseous environment.*

The main parameters used in the simulation are presented in Table 1.

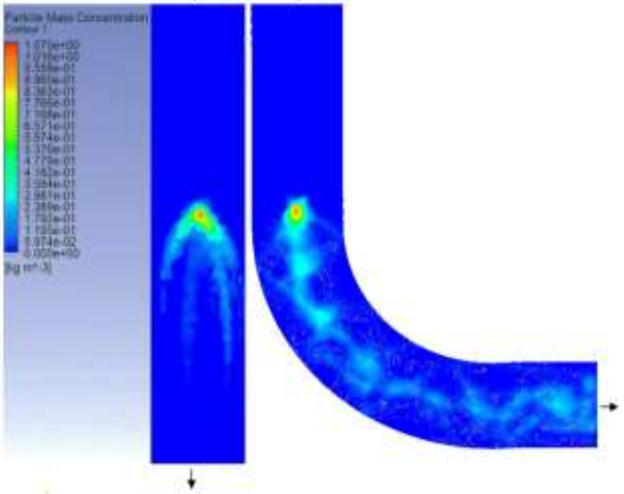
Table 1: *Parameters user for the simulation.*

Parameters	Value
Liquid temperature	293 K
Type of liquid	AdBlue
Density	1087 kg/m^3
Flow rate	75 x 10^{-6} kg/s
Gas temperature	700 K

3. Results and discussion

The following presents the results of the simulation of the AdBlue droplet vaporization process and the trajectories governing a droplet injected into a hot gaseous environment. As already mentioned the simulations have been performed for two exhaust pipe configurations in the same operating mode and compared with the analytical model.

Using the ANSYS Fluent simulation environment [9], using the two-equation ***k-epsilon*** model, in a continuous interaction environment, a drop of AdBlue having a flow rate of 0.0075 *kg/s* at a temperature of 293 *K* was considered to be injected into a gaseous environment of temperature 700 *K*.

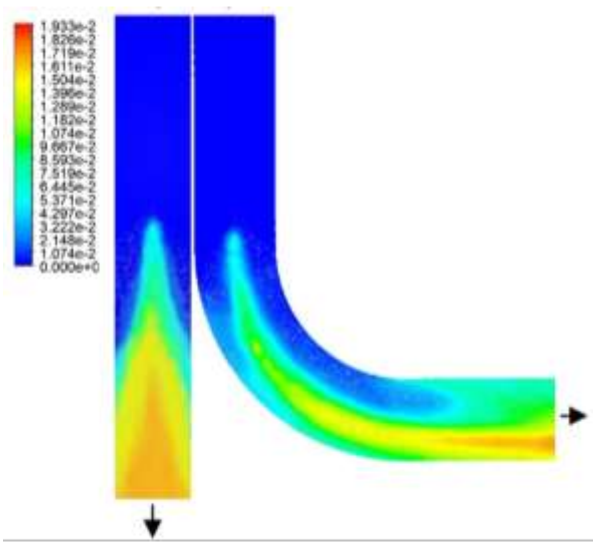


a) b)

Figure 5: *Diffusion of mass concentration in the case: a) straight pipe, b) 90° oriented pipe.*

In Fig. 5a) the diffusion of mass concentration in the gaseous environment as well as its dispersion due to gas flow in the straight configuration is analysed. In the case of the 90° oriented one, it can be seen in Fig. 5b) the appearance of turbulence from which it results that the liquid particles tend to evolve chaotically due to the diffusive phenomenon.

In Fig. 6 the evolution of the evaporation temperature of the single AdBlue droplet injected into the hot gas flow is observed.



a) b)

Figure 6: *Temperature contours and drop evolution over time.*

The mode of vapour diffusion in the gaseous environment is observed for the droplet in the 90° oriented duct. In this case the droplet is gradually vaporised so that it reaches the bottom of the pipe. In the case of straight channelling, the blue colour indicates the gas flow while the vapour resulting from the vaporisation of the droplet tends to occupy the entire volume during vaporisation.

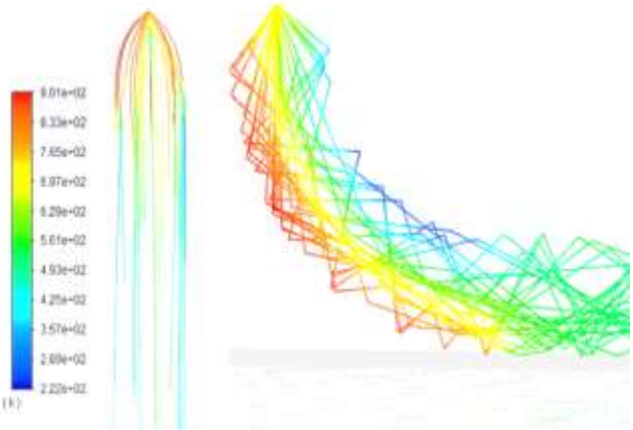


Figure 7: *Distribution of volume fractions for the two configurations.*

In Fig. 7 the distributions of the volume fractions of the two configurations can be observed, the substance droplet at the moment during vaporization at the contact between the gaseous environment.

4. Conclusions

In this study, it was shown in Fig. 2 plotted following a computational code made by the authors how a drop of AdBlue vaporizes in a gaseous environment at 700 *K* by analyzing the diameter over time. The results of the analytical calculations highlight that droplets with a smaller diameter evaporate faster because they provide more surface area per unit volume than larger droplets where evaporation occurs at the interface of the liquid and the gaseous environment. It was also found that there is a proportional dependence of the evaporation rate on time.

In order to study the vaporization mode and trajectory of a single AdBlue droplet, modeling in ANSYS using two different configurations of the hot gas flow channel was used.

It can be seen that at a gas temperature of 700 *K* the heat transfer between the liquid and gaseous environment is higher as the vaporisation rate increases, which will considerably affect the dispersion of the vapour and ultimately the cooling around the perimeter of the pipe.

For the two variants studied, it is observed that in the case of the configuration with a 90° oriented ducting, the gas velocity tends to increase and the particle trajectory generates a stronger diffusion moving chaotically, than in the case of the 180° oriented one. It can be deduced that the mixing of hot gases with fluid vapours is improved by increasing the heat transfer surfaces and orienting the flow direction at a 90° angle. Simulating the evolution of the vapour resulting from the vaporisation of an AdBlue droplet in a high temperature gaseous environment is the basis for understanding the processes of NO_x reduction using SCR systems.

5. Acknowledgment

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