

NUMERICAL INVESTIGATION OF THE BACK PRESSURE INFLUENCE ON UREA-WATER-SOLUTION MIXING PERFORMANCE IN CLOSE COUPLED SCR SYSTEM

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Abstract

The upcoming Euro 6d emission standard puts more even stringent requirements for diesel engine cars, especially in the case of nitrogen oxides (NO_x) emission. The most widely used technique to meet tight standards is Selective Catalytic Reduction (SCR) with urea-water-solution (UWS) injection. One of the crucial factors is even ammonia distribution at the catalyst inlet; hence, very often product development is focused around this issue. The product development is supported by both experimental and numerical work. The common approach to measure cross section ammonia distribution on the SCR is using sampling system at catalyst outlet. Very often exhaust layout is opened just after the SCR catalyst, cutting off the rest part for instance tailpipe or Clean-up Catalyst. Therefore, a backpressure at SCR outlet resulting from the downstream part is also eliminated. This could significantly affect flow parameters as the density changes, thus ammonia distribution and wall film deposition may vary as well. Within this work, the influence of the backpressure at SCR outlet on the ammonia distribution and wall wetting was numerically investigated. The simulations were run under various boundary conditions for the Close Coupled SCR architecture. It was shown that depending on the operating point the boundary pressure affects both factors on the different level.

Keywords: SCR, urea-water-solution, uniformity, CFD, back pressure

1. Introduction

Automotive diesel engine industry is facing now with successive emission regulations. The key issue is the nitrogen oxides (NO_x) limits. Recent Euro 6 regulations introduced another 55% NO_x reduction, from 180 mg/km to 80 mg/km for light duty cars, in comparison with Euro 5 norms [12]. Meeting such tight requirements needs exhaust gas after treatments systems as organizing combustion process exclusively is not sufficient enough. The most widely used technique is urea-water solution SCR system, as it stands out as very efficient way to NO_x abatement [7].

The urea-water solution (32.5% of the urea) is injected directly into hot exhaust gas stream and passing through water evaporation, thermolysis and hydrolysis produces ammonia – reducing agent [1]. To obtain high reduction efficiency, the crucial is to ensure even NH₃ distribution at catalyst inlet; hence, a lot of attention is paid for urea mixing itself. It becomes even more challenging with current SCR systems architecture standards that combine diesel particulate filter (DPF) with SCR functions in one volume what refers to selective catalytic reduction on filter (SCRoF). The SCRoF is usually placed downstream the diesel oxides catalyst (DOC) in possible close configuration with UWS injection between them [6]. Due to the packaging size, the distance between UWS injector and SCRoF inlet is not long enough to ensure proper UWS decomposition and NH₃ distribution. Therefore, the static mixing device is usually installed to enhance mixing process [10]. Nevertheless, this implies UWS-wall interaction and undesirable solid deposit formation may occur [2].

The product developing process is supported by both, CFD simulations and experiments. The literature reveals examples that show usefulness of CFD. For instance, simulations were used to improving mixer device in marine applications in case of mixing efficiency and pressure drop reduction [3] and mixing efficiency in vehicle application [11]. Simultaneously, a number of work was done in experiments. A different aspects were investigated as: NH_3 distribution [4, 8], deposit formation [9] and spray behaviour [5].

Very often to measure NH_3 distribution at the SCRoF outlet it is necessary to open layout in this place as shown in the [4]. Due to that, the whole under floor part is cut off, so if experiment is conducted in such configuration the SCRoF and upstream parts do not work in the same conditions as in the cars anymore as there is no backpressure at SCRoF outlet. Within this work, the sensitivity study of the backpressure at the SCRoF outlet influence on mixing and wall wetting performance was shown.

2. Simulations

Figure 1 presents close coupled DOC + SCRoF configuration. The geometry contains inlet, DOC, mixing cone, SCRoF and so called dummy outlet. Such layout refers to the prototype for the NH_3 distribution measurements at the outlet surface of the SCRoF. The system is opened just after the SCRoF to provide access for the gas-sampling ending, hence the working conditions are different comparing to those from the vehicle application. Cutting off the rest of exhaust system results in pressure change at the catalyst outlet as there is no backpressure from the under floor part anymore. To figure out how different is the performance of after treatment system with and without under floor part the number of test cases was simulated in the AVL Fire™ software. The calculations (Tab. 1) were performed for the different level of engine load assuming constant temperature of exhaust gases with two boundary conditions at the outlet for each load.

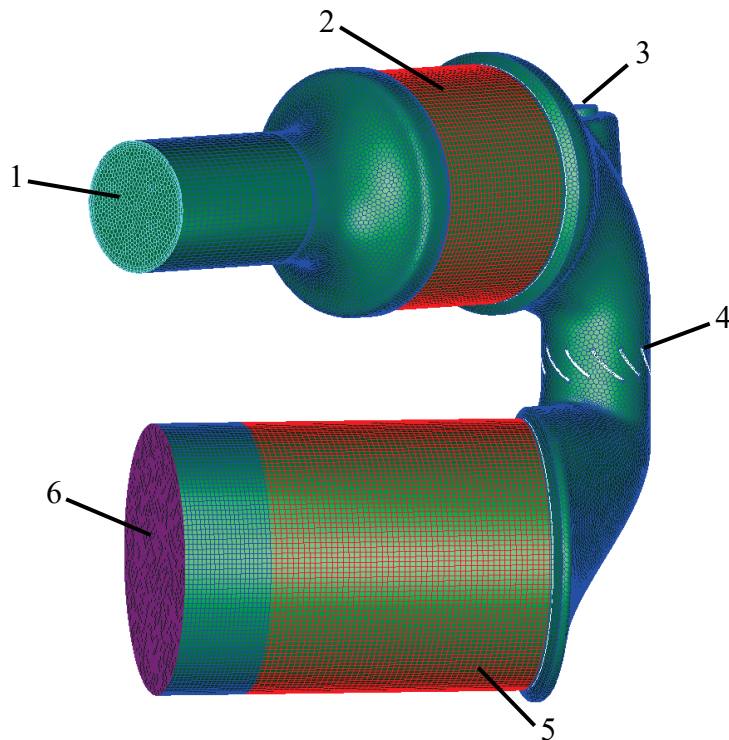


Fig. 1. Close coupled SCRoF system. 1 – inlet, 2 – DOC, 3 – injector, 4 – mixer, 5 – SCRoF, 6 – outlet

First, at each load the possibly outlet overpressure was calculated basing on quadratic pressure losses formula, what refers to the SCRoF outlet #1 in the Tab. 1 and simulates conditions similar

with those with complete exhaust system. The second pressure condition is atmospheric pressure for each load, what refers to SCRoF outlet #2 in the Tab. 1 and simulates the conditions that would occur with opened SCRoF. For each operating conditions the urea water solutions flow was calculated to maintain the NO_x to NH₃ ratio at stoichiometric level. With the mass load step of 10%, the total number of simulated cases was 20.

Tab. 1. Boundary conditions for calculation

Mass flow		Gas temperature	UWS	SCRoF outlet #1		SCRoF outlet #2
% load	[kg/h]	[°C]	[mg/s]	[-]	[kPa]	[-]
10	80	300	17.76	Atmospheric pressure +	0.70	Atmospheric pressure
20	160		35.54		2.73	
30	240		53.30		5.96	
40	320		71.08		10.19	
50	400		88.84		15.23	
60	480		106.61		20.91	
70	560		124.38		27.09	
80	640		142.15		33.66	
90	720		159.92		40.54	
100	800		177.69		47.65	

The mesh was built up by polyhedral elements on the inlet cone and mixing cone with the size fitted to cover properly the geometry curvature. Both, DOC and SCRoF were extruded from the mixing cone in order to obtain structural mesh on whole distance of catalysts. It can be seen in the Fig. 1, that dummy inlet and outlet were extruded also to provide stable boundary conditions. The total number of cells was of 567680.

3. Results

Figure 2 shows two main SCR system assessment benchmarks in function of mass flow. First is Uniformity Index (UI) at the SCRoF inlet given by equation 1, describing the NH₃ distribution:

$$UI = 1 - \frac{\sum_i |NH_{3i} - NH_{3avg}| \cdot A_i}{2 \cdot NH_{3avg} \cdot A_{Total}} \quad (1)$$

where:

NH_{3i} – mass fraction of the NH₃ at i- face,

NH_{3avg} – averaged mass fraction over the whole surface,

A_i – area of the i-face,

A_{Total} – total area of surface.

Second factor is film mass that remains at wall surface at the end of simulations. Both were represented as the relative value with the reference to the results obtains with the overpressure at the SCRoF outlet. In addition, at the same graph, the backpressure is shown in the same function. It can be seen that in whole mass flow range both factors have lower values for the atmospheric pressure outlet. For the mass flow range from 10% to 80% the relative UI, vary from 0.2 to 3.17 percentages points, and for wall film 0.6 to 2.7 percentage points. It means that lack of the backpressure for those operating points does not generate significant deviations in generated results.

However, after the 80% mass load there is a distinct drop of the both values. The decrease is over 10 and 22 percentage points for relative UI and wall film, respectively.

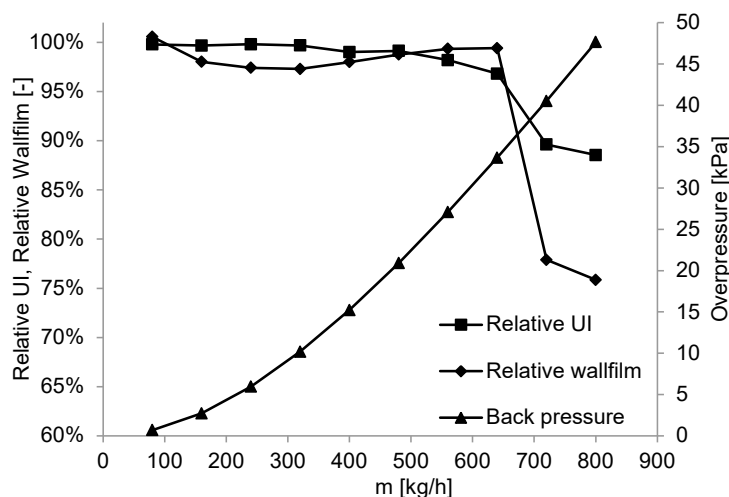


Fig. 2. Relative UI, Relative wall film and over pressure at SCRoF outlet in function of mass flow

The possible explanation for such situation is the density difference between tested cases starts to be crucial after some point. Along with the mass load, the difference between pressure inside the mixing cone increasing with the quadratic function, so the density as well. Here, the control value is the mass flow; it means that if there is no backpressure at the SCRoF outlet the velocity of the gas is higher than in the case with backpressure. Figs. 3-4 illustrate the velocity streamlines inside the mixing cone for the 80% and 100% mass load respectively. One can see that there is distinct velocity increase near the mixer area. In case of 80% load, the velocity range near the mixer varies from 82 m/s to 145 m/s with the applied backpressure, whereas for the atmospheric case the values are from 124 m/s to 185 m/s, and what is more, cover bigger volume. The averaged velocity value taken from section just after mixer is 117 m/s and 150 m/s. The differences are even more distinct for the 100% load. Here, in the averaged velocity taken from the same section are 132 m/s and 181 m/s respectively.

Such deviations could completely change the mixing process as well as the wall film evaporation. The higher value of the velocity means that urea water solution has less time for evaporation and for mixing with the exhaust gases, hence the noticeable UI decrease. Fig. 5-6 show the accumulated NH_3 that describe the time integrated molar flux trough the cell and could be treated as surface indicator of the ammonia distribution uniformity. At the Fig. 5 the map for 80% of load is shown, it could be noticed that the distribution without backpressure is slightly twisted counter clockwise. Moreover, due to the higher velocity, more NH_3 goes to the edge of catalyst and creates higher concentration level. Both scales are comparable, nevertheless the right picture presents wider range of scale, what again points out that the NH_3 high concentration region is fed at the cost of lower concentration region. The difference is even more distinct for the 100% load presented at the Fig. 6. At this operating point, the counter clockwise movement of the map is stronger. The NH_3 is concentrated on the smaller area that sticks to the left edge of the section. In addition, the scale differences are larger, the case without backpressure presents over five times higher value in the maximum points. The observed dependency is the main reason of UI differences between simulated cases. From the 90% mass load the velocity increase starts to completely redefine NH_3 distribution at the SCRoF inlet.

When considering wall film formation, due to the higher velocity, near the walls and wall film formation regions, there should be enhanced heat exchange between fluid and gas phases, hence also enhanced evaporation. Fig. 7 depicts wall film mass formation during one injection cycle. More mass is built up in the case of SCRoF outlet #1. Both characteristics reach maximum pick at the same time and start to evaporate. The difference at the top is lower that difference at the end of presented cycle. This point on faster evaporation process with the atmospheric outlet, what means that increased velocity near the walls affects evaporation characteristic.

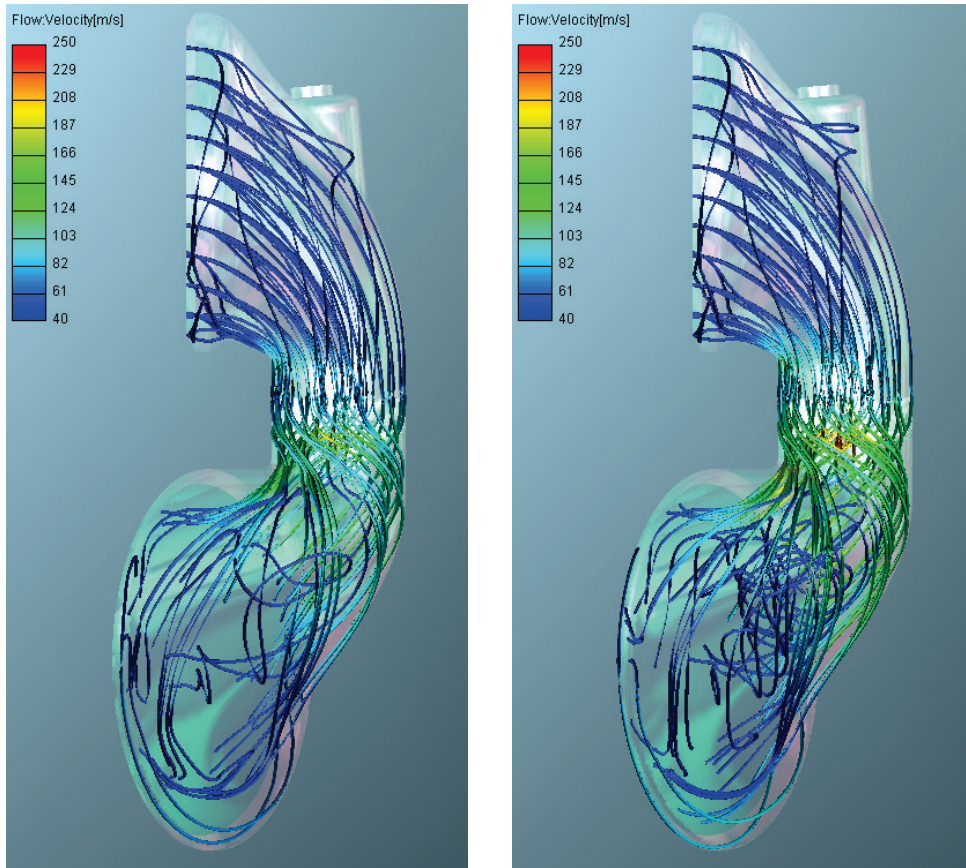


Fig. 3. Streamlines for 80% mass flow. Overpressure (left) and atmospheric (right) outlet

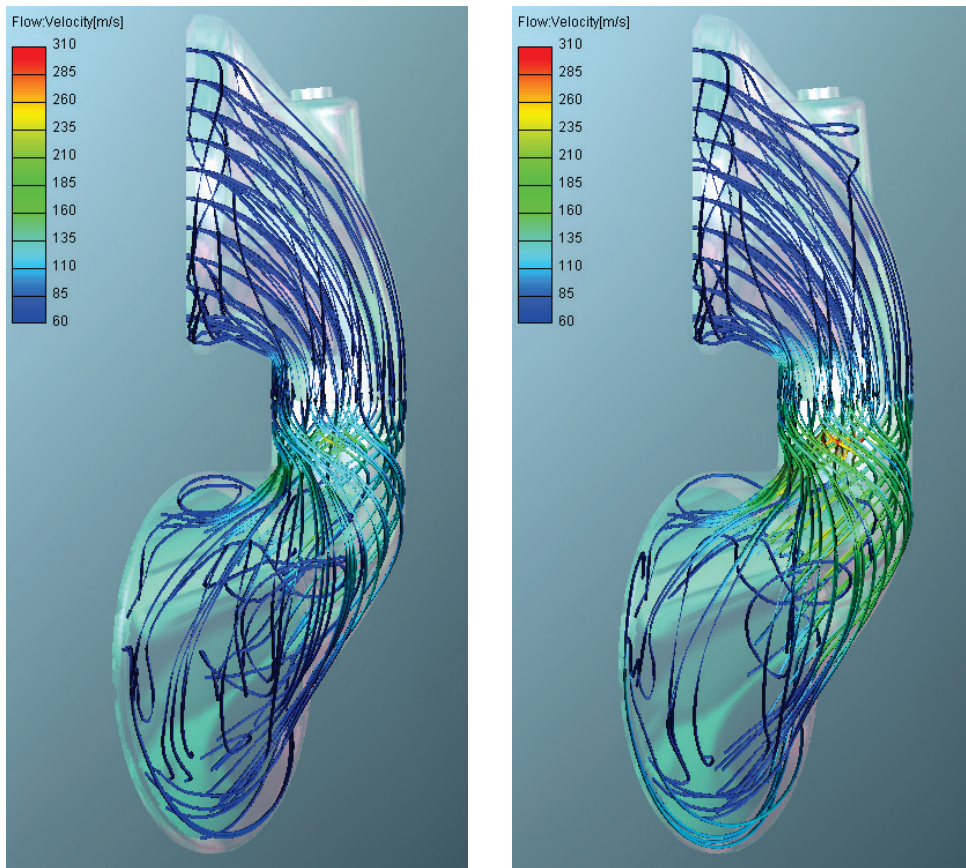


Fig. 4. Streamlines for 100% mass flow. Overpressure (left) and atmospheric (right) outlet

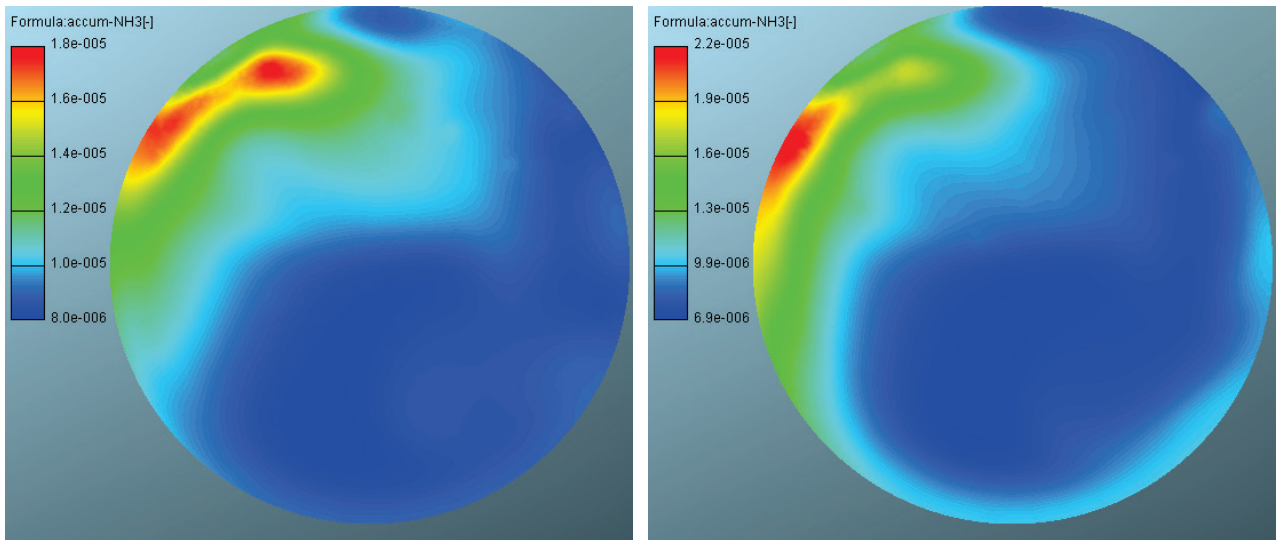


Fig. 5. Accumulated NH_3 at the SCRoF inlet for 80% mass flow. Overpressure (left) and atmospheric (right) outlet

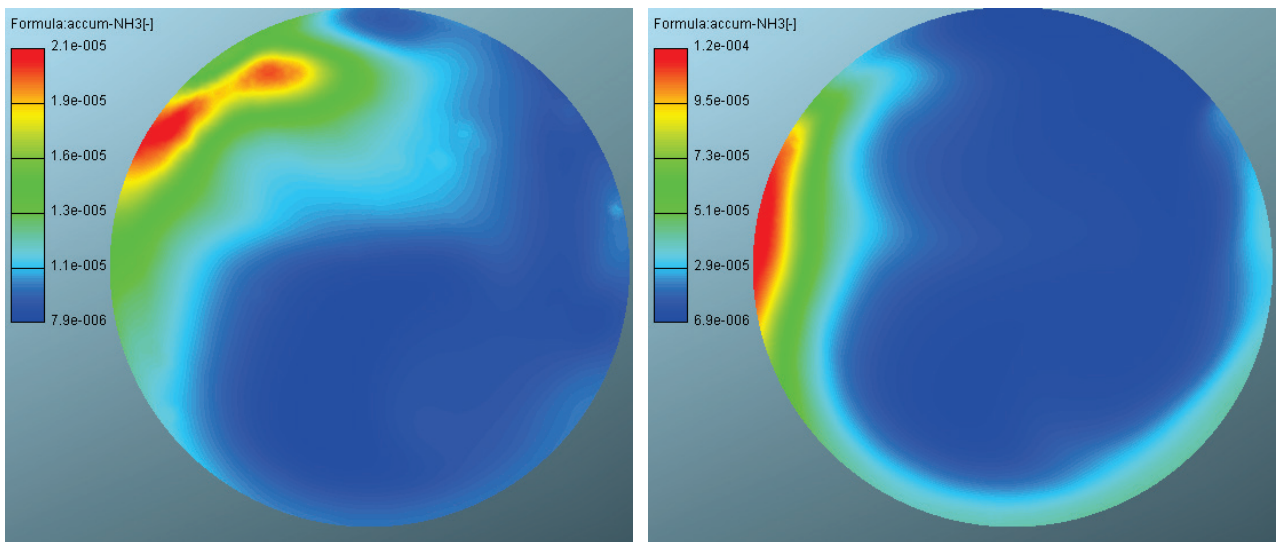


Fig. 6. Accumulated NH_3 at the SCRoF inlet for 80% mass flow. Overpressure (left) and atmospheric (right) outlet

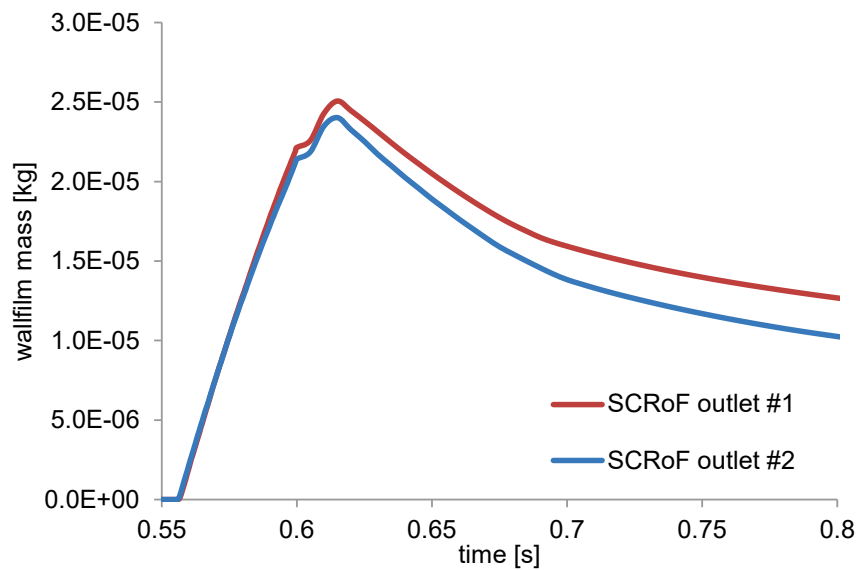


Fig. 7. Wall film mass formation during one injection cycle for 100% load

4. Conclusion

Within this work, the influence of the backpressure at SCRoF outlet on the system assessment benchmarks was investigated. The research showed that that depends on the back pressure both, Uniformity Index and wall film formation could perform different values. To some point, the distinction is at the low level and the results are not significantly affected. However, from the relevant conditions the difference start to be very distinct. In this case if once did not take into account the pressure deviation during the experiments, the outcome could be misinterpreted, as the conditions do not fully refers to real operating conditions.

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