COMPUTACIONAL SIMULATION OF THE EXHAUST GASES FLOW THROUGH A PLATINUM/PALADIUM CATALYTIC CONVERTER

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Abstract. *The study consists of a computational analysis of the exhaust gas flow through a Pt/Pd catalytic converter installed in an internal combustion engine run by ethanol. The values of energy and mass transport properties obtained in the experimental tests serve as initial values to the computational simulation developed by software CFX and MFIX. The programs shows a conservative equation group that allow pressure, temperature and velocity variation analysis of the exhaust gases along the monolithic support, besides evaluating the formation, emission levels from the combustion of incoming air-fuel mixture and its respective oxidation chemical reactions. The results of the simulation were compared to data obtained in the experiments.*

Keywords: *catalytic converter, engine, computational simulation, pressure drop.*

1. Introduction

The atmospheric air to hide every terrestrial crust this subjects to alterations in your chemical composition, due mainly, the presence of pollutant emissions generated by incomplete burning from the internal combustion engines, that produce high carbon monoxide, hydrocarbons and nitrogen oxides levels. The application of the catalytic converters in the automotive exhaust, added to the electronic injection system, contribute to assist thee maximum limits of gas emissions determined by PROCONVE (Programa de Controle da Poluição do Ar por Veículos Automotores). For the effective control of the vehicular emissions the automotive catalyst depends on the air-fuel massic flow, velocity and temperature exhaust gases.

According to Gunther et al (1988) in the regimes of the engine operation the flow from the burned gases through the exhaust system, causes load loss, due to the resistance of the flow through the mechanical components. The backpressure wave on the flow brings power loss and increase the engine fuel specific consumption's. In agreement with Chan (1999) the gas flow can be considered unidimensional through the automotive catalysts, which is composed by tiny channel that are isolated from each other.

The computational simulation of the exhaust gases flow by Pt/Pd catalytic converter is accomplished by two softwares: CFX for analysis of the hydrodynamic effects like variation of the speed and pressure along the catalytic converter, and MFIX that shows up the effect of the carbon monoxide and hydrocarbon oxidation chemical reactions along the monolith's channel.

2. Automotive Catalysts

The catalytic converter is a fundamental device in the reducing the exhaust levels emissions from automotive, formed by ceramic or metal substrates, where the gases drain through minuscule channels impregnated with precious metals (Pt and Pd) that accelerate the chemical reactions.

Figure 1. Components of the Catalytic Converter

The Fig. 1 shows the components of the automotive catalyst, which is composed by two monoliths that are involved by an expansible blanket, serving as thermal insulating and mechanical protection; and in the extremities they have cones denominated metal diffuser and mouthpiece, where in the inner part of the diffuser is a flow director to uniform the entrance of the gases flow in the monoliths. These components compose the catalytic converter.

Wark (1998) relates that the channel's walls of the monolith are catalytically inactive and permeated by a layer of metals of alumina oxides, cerium oxide and also zirconium oxide layer is increasing the contact surface. This process is denominated "washcoat ". A precious metals solution has distributed in the substratum surface. The Fig. 2 indicates the thickness of the wall (t) and the hydraulic diameter (Dh) of the monolithic channel.

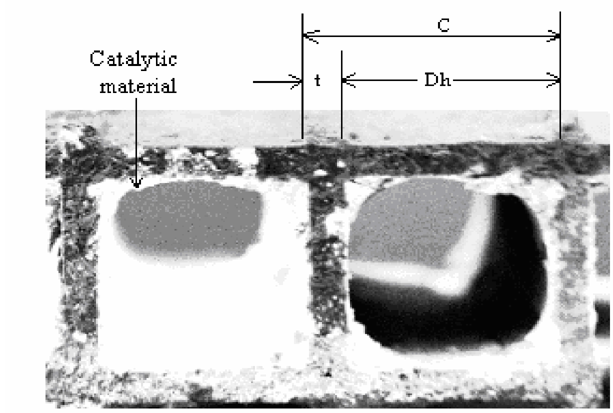

Figure 2. Dimensions of the monolith channel: t = 0,166mm, Dh = 1 mm e C =1,166mm

The catalytic converters has developed gradually in structure's resistance, improvement in the drawing, materials properties (promoting cells of high density that increase the contacts superficial area) and also besides the ceramic weight with fine walls for low heat capacity.

3. Materials and Methods

The outline of the tests bench is composed by a internal combustion engine, 4 cylinders run by ethanol, volumetric capacity of 1.987 liters, by Foucault's dynamometer (current type). In the system of the exhaust engine were installed 8 points for measurement of the pressure, temperature and gas flow. The microcomputer PC1 is applied together with a software ECM2001 for electronic injection control. The microcomputer PC2 works linked to a data acquisition system has done by the Workbench program, which indicates using thermocouples, the engine and the catalytic converter's temperature. The gases analyzer used it is of the NDIR typed - Infrared non Dispersive Analyzer. The measures of the gas pressures in the automotive catalyst have been done for two mmHg manometers, and the air pressure measured in the full mouthpiece it was accomplished for a mmH_2O manometer.

The operation conditions of the internal combustion engine were set to 50% on opening of the valve to a constant rotation of 1500 rpm. With I aid of the electronic manager ECM2001, the air excess factor was varied (λ) and keeping constant the ignition point. For the five sections of the automotive catalyst, that is, catalyst inlet pipe, support-1, empty, support-2 and the catalyst outlet pipe were measured the temperature, pressure, and also gases concentrations.

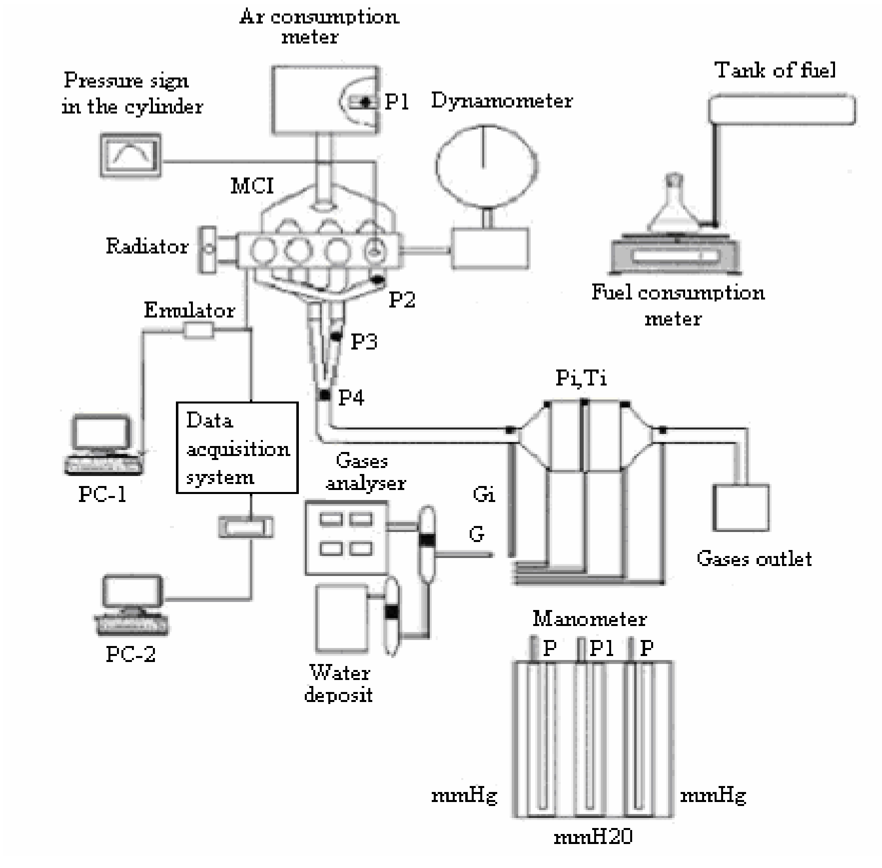

Figure 3 - Schematic Diagram of the Supported Experimental

According to Bejan (1984) The pressure drop in catalytic converter is treated by Fanning equation following:

$$\Delta P = \frac{2 f \rho V^2 L}{D_h} \tag{1}$$

Where, f - attrition -factor; ρ - density; V - speed; L- length; Dh - hydraulic diameter

Let us consider the attrition factor now for a laminate flow in duty of square transverse section, considered Eq. 2:

$$f = \frac{14{,}2}{\text{Re}} \tag{2}$$

The Reynolds number (Re) it is given as:

$$\mathrm{Re} = \frac{\rho V_1 D_h}{\mu} \tag{3}$$

The attrition factor for a turbulent flow the expressed form is:

$$f = \frac{0{,}3164}{\mathrm{Re}^{0{,}25}} \tag{4}$$

To apply the mathematical model of the exhaust gases flow along the automotive catalyst, the following hypotheses are adopted:

1 - average continue;
2 - steady state;
3 - incompressible flow;
4 – two-dimensional flow;
5 – k-epsilon turbulence model;
6 - disperse the lost by conduction, convection and irradiation energy transfer;
7 - there is not heat transfer through the catalyst walls.

The continuity equation.

$$\frac{d}{dx}(\rho u) + \frac{d}{dy}(\rho v) = 0 \tag{5}$$

The momentum conservation equations in the direction x and y.

$$\frac{d}{dx}(\rho uu) + \frac{d}{dy}(\rho vu) = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) \tag{6}$$

$$\frac{d}{dx}(\rho uv) + \frac{d}{dy}(\rho vv) = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial x}\left(\mu \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial y}\right) + \rho g \tag{7}$$

Species Transfer Balance Equation

$$\frac{\partial}{\partial x}(\rho u_j Y_i) + \frac{d}{dx}(\rho u_j Y_i) = -\frac{\partial P}{\partial x}(J_{i,j}) + R_i \tag{8}$$

The boundary condition needed for the solution of the species equation is following:

$$J_{i,j} = -\rho D_{i,m} \frac{\partial}{\partial x} Y_i \tag{9}$$

$$\frac{\rho}{M} K_{m,j} S(C_j - C_{s,j}) = R_j \tag{10}$$

Species Rate: R_j

$$R_j = -\delta S \gamma \sum_{K=1}^{N} a_{j,k} n_k r_k \tag{11}$$

Reaction Rate: r_k

$$r_k = \frac{A \ell^{\frac{-E}{RT}} C_A C_B}{G_1} = \frac{\bar{k}\, C_A C_B}{G_1} \tag{12}$$

Inhibition term

$$G_1 = T_S (1 + K_1 C_{CO} + K_2 C_{THC})^2 (1 + K_3 C_{CO}{}^2 C_{THC}{}^2)(1 + K_4 C_{NO}{}^{0,7}) \tag{13}$$

$$G_2 = T_S (1 + K_5 C_{CO} + K_6 C_{THC})^2 (1 + K_7 C_{CO}{}^2 C_{THC}{}^2)(1 + K_8 C_{NO}{}^{0,7}) \tag{14}$$

$$G_3 = T_S (1 + K_9 C_{CO} + K_{10} C_{THC})^2 (1 + K_{11} C_{CO}{}^2 C_{THC}{}^2)(1 + K_{12} C_{NO}{}^{0,7}) \tag{15}$$

Table 1. Reaction and reaction rate constants. Fonte: Koltsakis and Stamatelos (1999).

Reaction	Activation energy, E_i (J/mol)	Activity factor, A_i (mol K/m^2 s)	Constant, Ki	Adsorption heat, ΔH_i (J/mol)	Adsorption factor, A_k (mol K/m3 s)
$CO + 1/2\ O_2 \rightarrow CO_2$	90.000	1.4×10^{15}	$K_1 \rightarrow$	-7990	65.5
			$K_2 \rightarrow$	-3000	6430
$H_2 + 1/2\ O_2 \rightarrow H_2O$	90.000	1.4×10^{15}	$K_3 \rightarrow$	-96534	3.98
			$K_4 \rightarrow$	31036	47900
$CxHy + \alpha O_2 \rightarrow \beta CO_2 + \gamma H_2O$ (slow HC)	105.000	3×10^{14}	$K_5 \rightarrow$	-7990	400
			$K_6 \rightarrow$	-3000	25700
			$K_7 \rightarrow$	-96534	3.98
$CxHy + \alpha O_2 \rightarrow \beta CO_2 + \gamma H_2O$ (fast HC)	125.000	4×10^{14}	$K_8 \rightarrow$	31036	47900
			$K_9 \rightarrow$	-7990	400
			$K_{10} \rightarrow$	-3000	200
$CO + H_2O \rightarrow CO_2 + H_2$	105.000	6×10^{8}	$K_{11} \rightarrow$	-96534	3.98
			$K_{12} \rightarrow$	31036	200000
$CO + NO \rightarrow 1/2N_2 + CO_2$	70.000	5×10^{6}			

According to Pontikakis (2003) the diffusion and reaction problem on washcoat wall has solution through of the CO and THC species transfer balance equation as follow:

$$-\frac{\partial P}{\partial x}\left(J_{i,j}\right)+R_i=0 \tag{16}$$

$$-\frac{\partial}{\partial x}\left(-\rho D_{i,m}\frac{\partial}{\partial x}Y_i\right)+\frac{\rho}{M}K_{m,j}S(C_j-C_{s,j})=0 \tag{17}$$

For (CO and THC) the species transfer balance equation become:

$$D_{eff}\frac{d^2Y^{CO}}{dx^2}+\frac{Kb_1}{G_{red2}}Y^{CO}Y^{O_2}=0 \tag{18}$$

$$D_{eff}\frac{d^2Y^{HC}}{dx^2}+\frac{Kb_2}{G_{red1}}Y^{HC}Y^{O_2}=0 \tag{19}$$

Where $Kb_i = k / D_{eff}$; $\Delta Y_o = Y_o^{O2} - 0{,}5Y_o^{CO}$; $\Delta Y_o = Y_o^{O2} - 3{,}5Y_o^{HC}$; $G_{red1} = (1 + K_2Y^{HC})^2$; $G_{red2} = (1 + K_1Y^{CO})^2$.
The solution of the equation (20) and (21), through the routines in language FORTRAN applied and in the program MFIX as term source in the channel wall.

$$\frac{dY^{CO}}{dx}=-(Kb_1(U_1-U_2-U_3)+2Kb_1\Delta Y_o(U_4+U_5))^{1/2} \tag{20}$$

$$\frac{dY^{HC}}{dx}=-(7Kb_2(U_1-U_2-U_3)+2Kb_2\Delta Y_o(U_4+U_5))^{1/2} \tag{21}$$

4. Results

The THC, CO and NOx emissions along the catalyst are shown in Fig. 4, in operating condition of the internal combustion engine set to 50% on opening of the valve, in the rotation of 1500 rpm, and with an air excess factor 0,94, it was observed a reduction of 100% of the NOx emission in the first monolith (S-1). While the oxidation THC and CO emissions, in the catalyst outlet, was not satisfactory according to the maximum limit required by PROCONVE.

In same operating condition of the engine the temperature, pressure and gas flow vary along the catalyst with air excess factor, as shown in Fig. 5, the configuration of the electronic injection engine was altered by the software ECM2001, it was observed that with the decrease of time of fuel's injection, by the impoverishment methods, it has resulted in the decrease of the gas flow, due to lower presence of mass of fuel. The temperature and the pressure had the same tendency, starting from the air excess factor 0.98 they decreased with the more poor mixture.

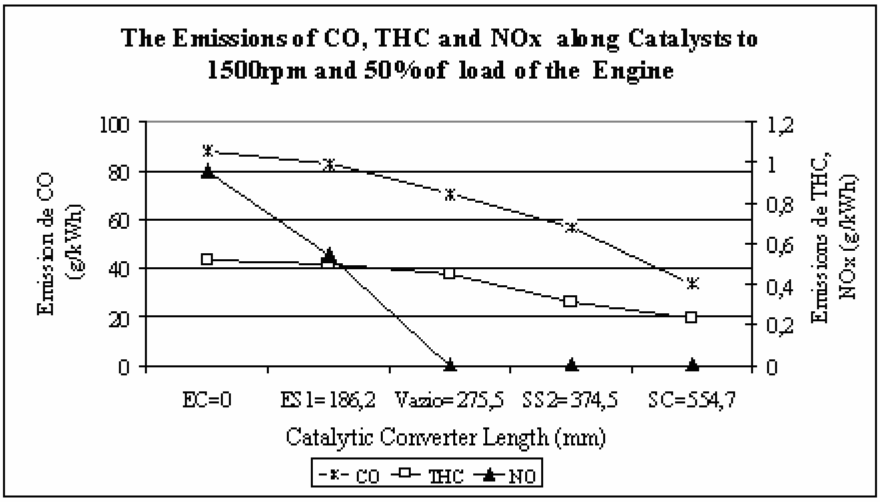

Figure 4. CO, THC and NOX emissions along the catalytic converter

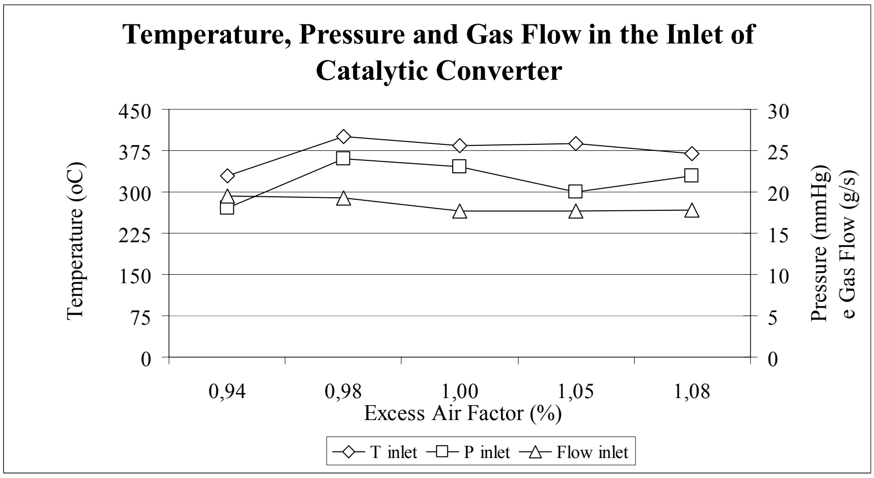

Figure 5. Temperature, pressure and gas flow of the exhaust gases in the catalysts inlet

The Fig. 6 shows the pressure variation along the exhaust system, in same operation condition of the engine, without altering the normal configuration of the engine electronic control, it was observed two pressure peaks, the first corresponds to the ramification junction of the exhaust collector and the second located peak in the first monolith inlet, due to the diffuser, that reduces the velocity with increase of the pressure, and for the resistance of the monolith.

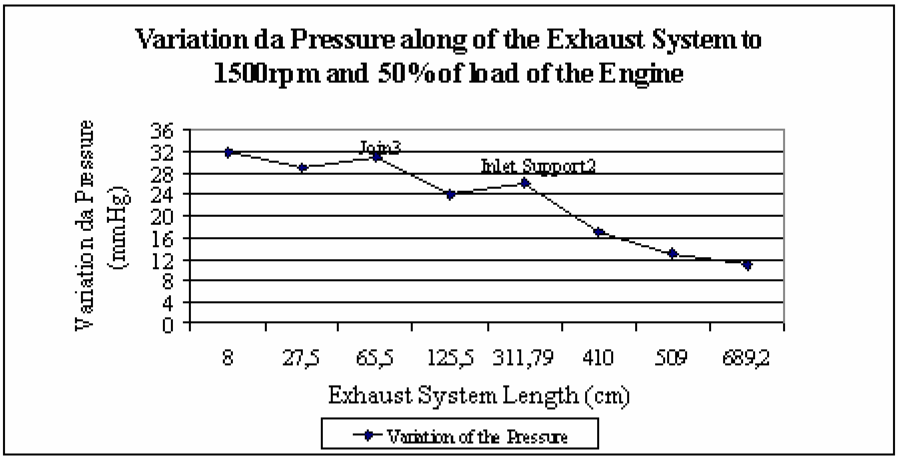

Figure 6. Pressure variation along the exhaust system of the internal combustion engine

The Fig. 7 shows the velocity and pressure variation along the catalytic converter. The application of the software CFX indicates the hydrodynamic effects of the exhaust gases in steady state and with two-dimensional flow. In the

Fig. 7 the value of the velocity in outlet is maximum, because the plan is located in the center of the catalytic converter. The medium simulated velocity in the catalyst outlet was of 19,53 m/s, near to the medium value obtained experimentally 19,29 m/s. And also in Fig. 7 have been observed the graphs of dynamic behavior of the velocity variation and gases pressure variation in the exhaust.

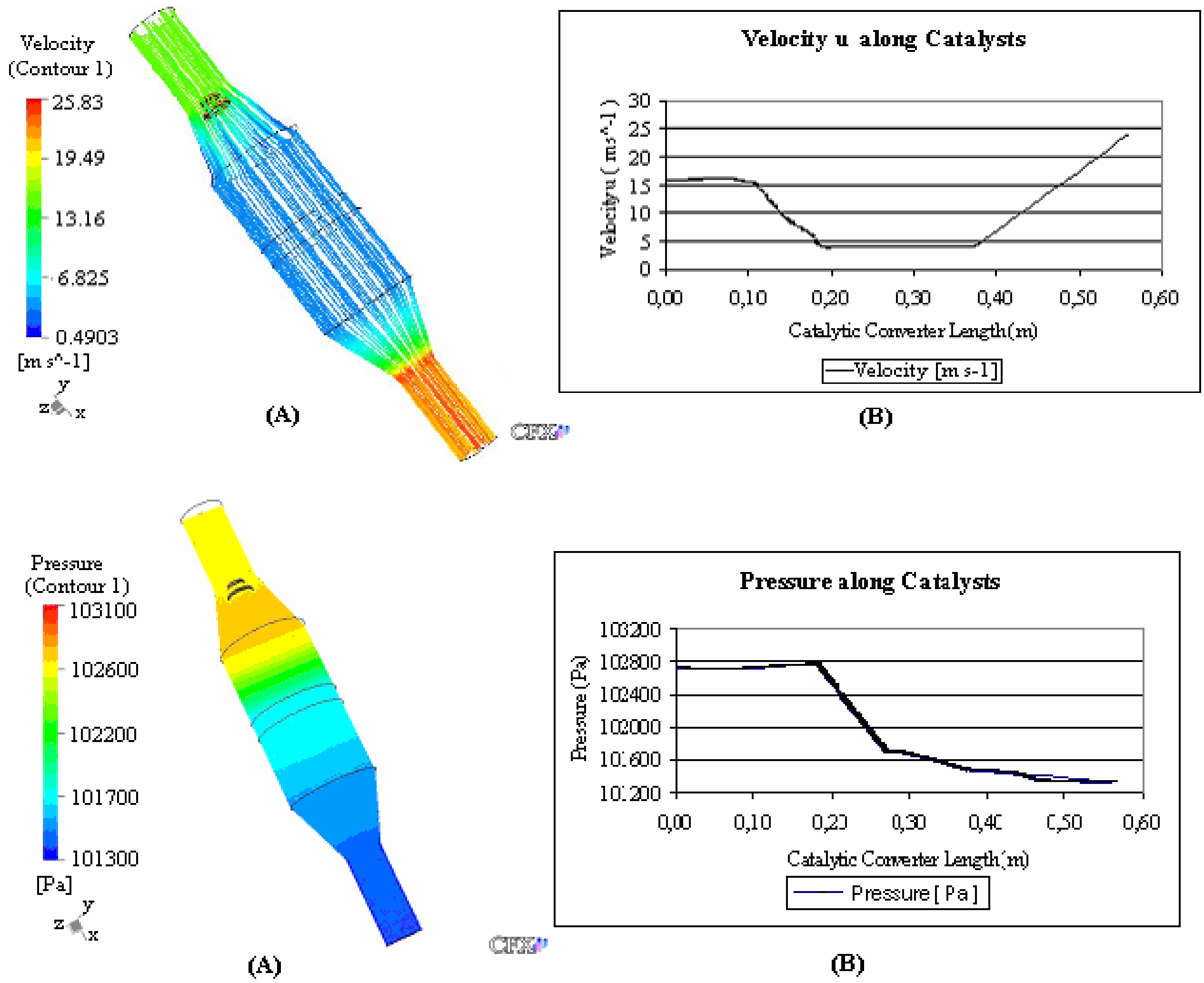

Figure 7. Simulation of the velocity and pressure variation along the catalytic converter

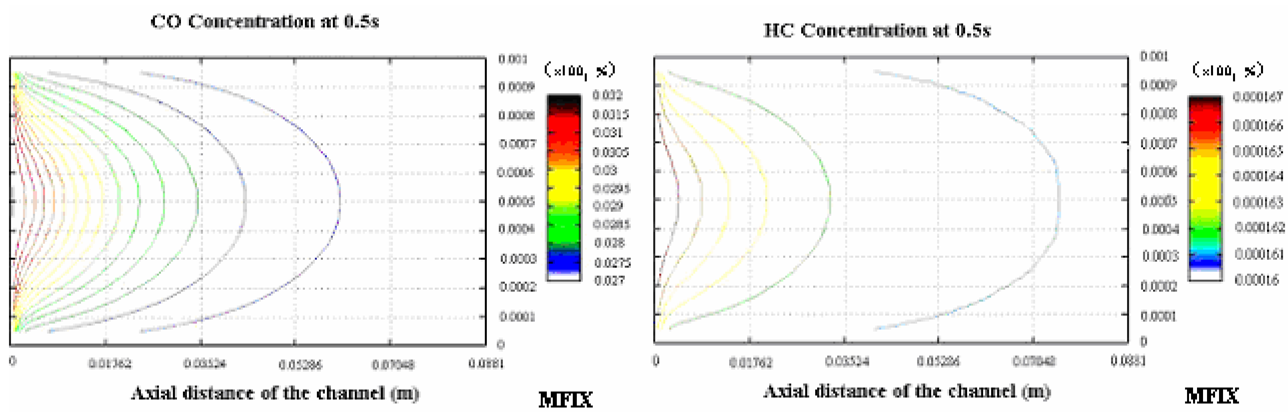

Figure 8. CO and HC concentration at 0,5seg along the channel

The Fig. 8 indicates the reactions simulation of the oxidation's reactions of carbon monoxide and hydrocarbon from the exhaust gases, through the first monolith channel of the catalytic converter. The inlet initials values for the simulation result of the experimental data. The operation's conditions of the engine were set to 50% on opening of the valve, constant rotation of 1500 rpm and air excess factor (λ) equal to 0,94. The software MFIX allowed the chemical treatment of the gases reactions along a single channel, as well as in the analysis of the chemical reactions behavior in the channel surface, being applied sources terms in the channel wall, that they correspond to the catalyzes of the chemical reactions.

The implementation of the source term was developed by FORTRAN program and soon after adapted in the boundary condition of the MFIX software. The experimental medium values measured of the CO and THC species by gases analyzer NDIR, in the first monolith outlet were 2,70% and 153 ppm, respectively, and also the respective medium values of the species CO and THC obtained in the simulation computational were 2,72% and 160 ppm.

The Fig. 9 shows the variation of the gases chemical reaction along the channel in five indicated positions among the center of the channel and near to the wall surface. It has been verified that the more near of the wall, as in the CO position p0,1mm, tends to accelerate the chemical reaction process. In the central position (COp0,5mm) occurs lower influence of the catalytic effect of precious metals.

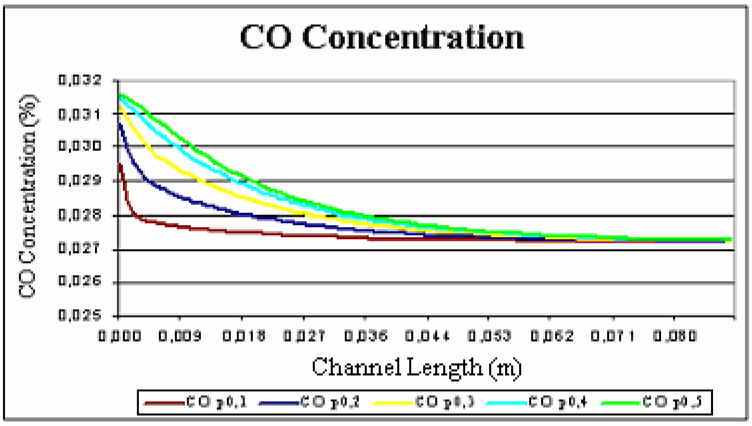

Figure 9. CO concentration in five position of the channel

5. Conclusions

The application of the CFX and MFIX software contribute to analysis detailed of the hydrodynamics and chemical reaction effect in flow exhaust. It was verified a difference of 1.23% between the experimental and simulated average velocity. Moreover for CO and HC species it was observed a difference of 0.74% and 4.5%, respectively.

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