ANALYSIS OF THE OXIDATION REACTIONS IN EXHAUST GASES ALONG OF A MONOLITHIC CHANNEL

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Abstract. *The work describes computational analysis of the exhaust gases flow through a Pt/Pd catalytic converter installed on internal combustion engine fueled by ethanol. The hydrodynamic effect and the chemical reactions of the exhaust gases flow have computationally simulated employing itself the software MFIX. The program solves a group of conservative equations that allow to analysis of the physical-chemical property variation of exhaust gases along of a monolithic channel single. In computational simulation of the monolithic channel applied itself the process of the refinement of grid and a comparative between the Foup, Van Leer e Superbee scheme numeric with many grid.*

Keywords: *automotive catalysts; emission control; hydrodynamic and chemical simulations.*

1. Introduction

The modern society applies process of combustion of the materials for energy attainment and execution of work in its daily activities. The energy produced world-wide for the combustion process is almost all consumed in the great rich urban centers and countries, that emit high levels of toxic substances to the atmospheric environment, resulting in the deterioration of the ambient conditions and considerable change of the normal concentrations of gases of the troposphere.

The formed pollutants of the combustion in the internal-combustion engines (ICE) are: monoxide of carbon (CO), hydrocarbons (HC), nitrogen oxides (NOx), oxides of sulphur (SOx), particles (PM), aldehydes (CHO), beyond harmless substances as vapor of the water, nitrogen and the dioxide of carbon (CO2), this last gaseous component, even so either considered as a pollutant of low toxicity, must be taken in consideration, in view of its participation in the "effect greenhouse".

The treatment of the pollutant emissions was improved with application of the catalytic converter that chemically reduces the pollutants contained in the exhaust gases, through heterogeneous catalytic reactions of oxidation and reduction in the surface of the monolith, allowing to the species of the exhaust gases to spread out inside of the catalytic material or "washcoat". The presence of precious metals as: platinum, palladium and ródio speed up the process of the reactions of reduction of nitrogen oxides and oxidation of the carbon monoxide and hydrocarbons in the surface of the walls for the center of the monolithic channel.

In present work was implemented and resolved mathematical model that describes the chemical reactions in the surface of the monolith by means of the software MFIX, that resolve the equations of rocking of species for the diffusion and reaction in the catalytic material, by means of the application of a source term or equation of contour in the catalytic surface throughout a simple channel of the monolith.

The source term was implemented in a program of FORTRAN language, called automotive catalytic program for species THC and CO, which resolve the problem of diffusion-reaction in the catalytic material, using the method runge-kutta in the resolution of the different mathematical formularizations of the catalysis in the exhaust gases. The draining verified through the monolith is laminar, had to the low Reynolds number. The values of the border conditions had been adopted by the gotten data experimentally.

2 - Channel of the Monolith

Wark (1998) relates that the channel walls of the monolith are inactive catalytically and permeated of the alumina oxide metal layer, cerium oxide layer and also zirconium oxide layer, that increases the contact surface. This process is denominated "washcoat ". It is distributed in the surface of the substratum a precious metals solution. The Figure 1 and Figure 2 indicate the thickness of the wall (t) and the hydraulic diameter (Dh) of the monolithic channel.

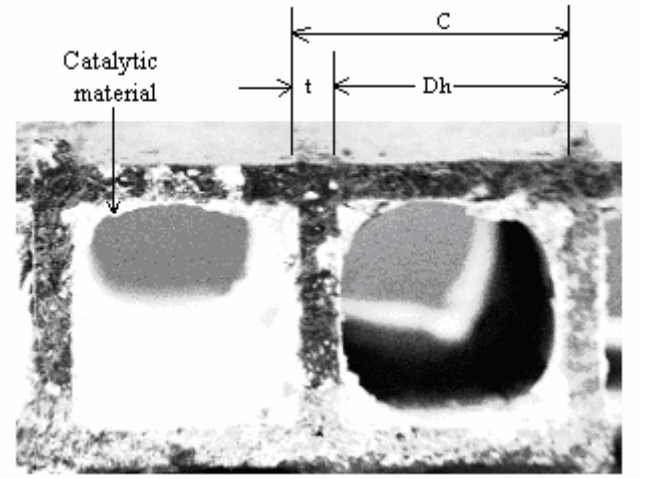

Figure 1 – Dimensions of the channel of the monolith: t = 0.166mm, Dh = 1 mm e C =1.166mm

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

3 - Modeling of the Monolith Channel.

The two-dimensional model of the draining of the gases burnt for a simple monolithic channel was developed in the software MFIX that allowed analyzing the transference of mass and the chemical reactions of oxidation of the exhaust gases along of a channel. The effect of the diffusion-reaction in the wall of the channel covered with catalytic material was described with the implementation of a source term as condition of border developed in the Catalytic program Automotive. Some hypotheses had been adopted as half continuous, two-dimensional draining, steady state, fluid incompressible, laminar draining, disdained the heat transferences.

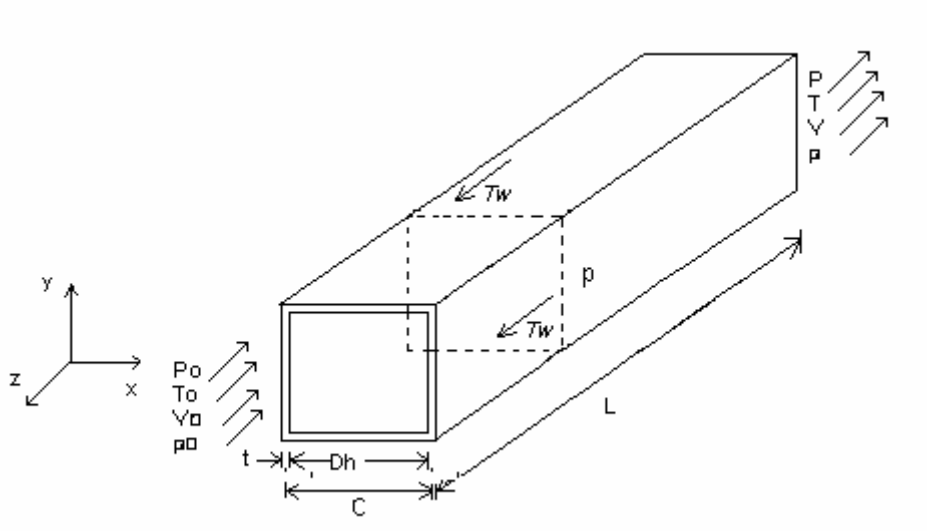

Figure 2 – Dimensional in monolith cellule.

Code MFIX was developed to simulate draining gas-solid in stream fluidize beds, considering chemical reactions, however it was adapted to decide the problem of chemical catalysis of the draining of the exhaust gases in a simple channel of the monolithic support of the automotive catalysts. However, the function of the properties of the solid phase

was incapacitated in the programs of simulation for oxidation of THC and CO. Code MFIX uses mesh of the structuralized type and the method of finite volumes.

According to Ciola (1981), the reaction of the exhaust gases on the catalytic surface occurs way molecular diffusion, by means of events, such as: diffusion of the reagents until the surface (mass transport interface) and for inside of the pores (mass transport intraface), adsorption of the reagents on the surface, dessorption of the products, diffusion of the products for are of the pores and for inside of the chain of the fluid.

A hundred of reactions occur simultaneously on the surface of the catalysts and enter some chemical species of the exhaust gases. The reactions associates to the oxidation processes are the following ones:

Table 1. Reaction considered in the mathematical model and the reaction rate constants.
Source: Pontikakis et al (2001)

Reaction	Activation energy, E_i (J/mol)	Activity factor, A_i (mol K/m2 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	$1.4x10^{15}$	$K_1 \rightarrow$	-7990	65.5
			$K_2 \rightarrow$	-3000	6430
$H_2 + 1/2\ O_2 \rightarrow H_2O$	90.000	$1.4x10^{15}$	$K_3 \rightarrow$	-96534	3.98
			$K_4 \rightarrow$	31036	47900
$CxHy + \alpha O_2 \rightarrow \beta CO_2 + \gamma H_2O$ (slow HC)	105.000	$3x10^{14}$	$K_5 \rightarrow$	-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	$4x10^{14}$	$K_8 \rightarrow$	31036	47900
			$K_9 \rightarrow$	-7990	400
			$K_{10} \rightarrow$	-3000	200
$CO + H_2O \rightarrow CO_2 + H_2$	105.000	$6x10^{8}$	$K_{11} \rightarrow$	-96534	3.98
			$K_{12} \rightarrow$	31036	200000
$CO + NO \rightarrow 1/2N_2 + CO_2$	70.000	$5x10^{6}$			

To apply the mathematical model of the flow of the exhaust gases along of the monolith channel, according to Chan (1999) and Braun et al (1999), the following hypotheses are adopted:

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

Species Transfer Balance Equation

$$\frac{\partial}{\partial x}\left(\rho u_j Y_i\right) + \frac{d}{dx}\left(\rho u_j Y_i\right) = -\frac{\partial P}{\partial x}\left(J_{i,j}\right) + R_i \tag{1}$$

The boundary conditions needed for the solution of the species equation are following:

$$J_{i,j} = -\rho D_{i,m} \frac{\partial}{\partial x} Y_i \tag{2}$$

$$\frac{\rho}{M} K_{m,j} S(C_j - C_{s,j}) = R_j \tag{3}$$

Species Rate: R_j

$$R_j = -\delta S \gamma \sum_{K=1}^{N} a_{j,k} n_k r_k \tag{4}$$

Reaction Rate: r_k

$$r_k = \frac{A\ell^{\frac{-E}{RT}} C_A C_B}{G_1} = \frac{\bar{k} C_A C_B}{G_1} \tag{5}$$

Inhibition term

$$G_1 = T_S(1 + K_1 C_{CO} + K_2 C_{THC})^2 (1 + K_3 C_{CO}{}^2 C_{THC}{}^2)(1 + K_4 C_{NO}{}^{0,7}) \tag{6}$$

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

$$G_3 = T_S(1 + K_9 C_{CO} + K_{10} C_{THC})^2 (1 + K_{11} C_{CO}{}^2 C_{THC}{}^2)(1 + K_{12} C_{NO}{}^{0,7}) \quad (8)$$

The diffusion and reaction problem on "washcoat" wall has solution through of the CO and THC species transfer balance equation as follow:

$$-\frac{\partial P}{\partial x}\left(J_{i,j}\right) + R_i = 0 \quad (9)$$

$$-\frac{\partial}{\partial x}\left(-\rho D_{i,m}\frac{\partial}{\partial x}Y_i\right) + \frac{\rho}{M}K_{m,j}S(C_j - C_{s,j}) = 0 \quad (10)$$

According to Pontikakis (2003) for species CO e THC the species transfer balance equation become:

$$D_{eff}\frac{d^2Y^{CO}}{dx^2} + \frac{Kb_1}{G_{red2}}Y^{CO}Y^{O_2} = 0 \quad (11)$$

$$D_{eff}\frac{d^2Y^{HC}}{dx^2} + \frac{Kb_2}{G_{red1}}Y^{HC}Y^{O_2} = 0 \quad (12)$$

Where,
$Kb_i = k / D_{eff}$; $\Delta Y_o = Y_o{}^{O2} - 0.5Y_o{}^{CO}$; $\Delta Y_o = Y_o{}^{O2} - 3.5Y_o{}^{HC}$; $G_{red1} = (1 + K_2 Y^{HC})^2$; $G_{red2} = (1 + K_1 Y^{CO})^2$.

The solution of the equation (11) and (12), through the routines in FORTRAN language applied and using the program MFIX as source term in the wall of the channel.

$$\frac{dY^{CO}}{dx} = -(Kb_1(U_1 - U_2 - U_3) + 2Kb_1\Delta Y_o(U_4 + U_5))^{1/2} \quad (13)$$

$$\frac{dY^{HC}}{dx} = -(7Kb_2(U_1 - U_2 - U_3) + 2Kb_2\Delta Y_o(U_4 + U_5))^{1/2} \quad (14)$$

According to Martins (2006) in the entrance of the monolithic channel for simulation of the carbon monoxide and hydrocarbon oxidation chemical reactions with software MFIX, is had: the concentrations of the gases of 3.17% CO, 0.24% O_2, 12.6% CO_2, 167ppm HC, 193ppm NOx; e the thermodynamic properties: T = 645 K; P = 102524.97 Pa; V = 3.84 m/s.

The condition of border in the outlet of the catalytic converter is given by the pressure, P = 1atm or 101325 Pa and ambient temperature, T=300 K.

The source terms of the species catalyzed developed in the automotive catalysts program had been adapted as contour conditions in the simulation of software MFIX in the walls of a simple channel, the result was:

$\dot{\dot{Y}}_{HC} = 0.0001609$ e $\dot{\dot{Y}}_{CO} = 0.0270232$.

4 – Methodology.

The internal-combustion engine (ICE) ran with 50% of opening of the butterfly and the rotation of 1500rpm for all the collections of gases in the automotive catalysts, installed in the exhaust system of a GM engine fueled by ethanol, 4 cylinders, 1.998 liters of total piston displacement and 12:1 of compression rate. Three taking of gases placed in the automotive catalysts is connected to the analyzer of gases, these taking is constituted by a copper pipe of 10mm of diameter and 350mm of length. After 3 minutes of functioning of the ICE, the measures of the concentrations of gases in the catalysts had been initiated, obeying themselves a sequence of the taking of gases: entrance of support 1, emptiness and finally exit of support 2. An interval of 1 minute was established enters the acquisitions of the samples, without alteration of the opening of the butterfly and rotation of the ICE, until the attainment of the 10 samples.

The 10 samples of the concentrations of CO, THC, NOx, CO_2 and O_2 had been treated statistics, to determine the interval of uncertainty in the measurement ($\pm\delta x_i$), that it can be represented by the eq. (15).

$$x_i = x_i(medida) \pm \delta x_i \quad (15)$$

In the measurement of the concentrations of the gases of the exhaust system the analyzer of type NDIR used itself, Analyzer Infra-red not Dispersive, for measurement of the concentrations of monoxide of carbon, hydrocarbons, oxygen, dioxide of carbon and nitrogen oxide, being the measurements carried through for an equipment with specific

characteristics for measurement of emissions of the automotive line. However, the measurements of hydrocarbons had been gotten also using the analyzer of the type FID, Detector of Ionization of Flame.

As Heywood (1986) the analysis of the majority of the exhaust gases is made by devices standards such as: 1º) FID, that corresponds to an efficient carbon accountant, or either, the hydrocarbons contained in the exhaust gases are burnt in a small air-hydrogen flame, having produced ion in a proportional amount to the burnt carbon atom number. 2º) NDIR, in which occurs absorption for infra-red ray of the hydrocarbons in a cell of sample of the gases of the exhaustion, that are compared by the absorption of a cell of used reference to determine this concentration. The values of hydrocarbons measured for analyzer FID are approximately two times the value measured in analyzer NDIR.

For the measures of repeatability of the collection of the CO emissions, THC and NOx, CO2 and O2 through out 3 positions of the catalytic converter had been affected in 10 samples for each position of the converter.

Table 2 – Calculation of uncertainty of the exhaust emissions.

Concentration Exhaust Gases	inlet Support 1	Void	Out Support 2
CO	3.17±0.04	2.7±0.03	2.19±0.02
THC	167±2	153±2	106±1
NOx	193±3	0	0
CO_2	12.6±0.3	13±0.2	13.3±0.4
O_2	0.24±0.02	0	0

Software MFIX allows the chemical treatment in the draining of the gases of the exhaustion, as well as the analysis of the behavior of the chemical reactions in the surface of a simple monolithic channel. A source term is applied as condition of border in the surface of the wall of the channel, causing the effect of catalyzes associated to the chemical reaction and diffusion of the gases.

Table 3 – Parameters of Simulation in a simple monolithic channel using MFIX code.

Parameters of Computational Simulation using MFIX code			
Mesh	Method Numeric	Total Time Condition for Simulation	Processing Time of the CPU
100x10	Foup	1 s	1day 1hours
100x10	Van Leer	1 s	1day 7hours
100x10	Superbee	1 s	1day 11hours
220x10	Foup	1 s	3days 11hours
220x10	Van Leer	1 s	4days 17hours
220x10	Superbee	1 s	2days 9hours
440x20	Foup	1 s	26days 13hours

The initial values for the simulation result of carried through experimental data in suporte1. The operational conditions of the engine had been fixed in 50% of opening of the butterfly, 1500rpm and with factor of air excess (λ) equal the 0.94. The physical largeness as: temperature, pressure, speed and concentration of the gases had been measured in the entrance of the monolithic support and estimates as initial conditions for the simulation.

The implementation of the source term was developed in a program of FORTRAN language, and later adapted as condition of border in software MFIX. In the exit of the first one it has experimentally supported the gotten average values of the species of CO and 153 THC had been 2.70% and 153ppm, respectively. While, in the computational simulation the average values of the species had been of 2.72% of 160 CO and 160ppm of THC.

5 - Results.

The monolithic support of the catalytic converter consists of innumerable channels for where their drain the burnt gases, these channels allow chemical reactions of catalyze in its surface. If the diameter of the channel to increase, will cause to reduction of the loss of load, benefiting bigger volumetric efficiency in the engine with consequent increase of the

power, however the catalytic efficiency in the automotive catalysts can be reduced and the emissions to pass not to take care of to the maximum limits established by the PROCONVE (Program of Control of the Pollution of Air for Automotive Vehicles).

The Figure 3 indicates the simulation of the chemical behavior of the gaseous reactions in the decurrently channel of the variation of the diameter. For the normal diameter of the channel of 1mm the emission of carbon monoxide simulated in the outlet of the channel was of 2.7%, when the diameter of the channel was increased gradual until 2mm, an esteem loss of 7.4% in the catalytic efficiency of the automotive catalysts was observed approximately. In this simulation as the diameter of the channel it varied of 1mm for 2mm, was kept constant a ratio of the mesh of 8.809 exactly having varied its diameter.

The reason of the spacing of the mesh in x,y.

$$\frac{\Delta y}{\Delta x} = \frac{10}{100} = 0.1$$

The dimension of channel in x and y.

$$\frac{\Delta y}{\Delta x} = \frac{1mm}{88.091mm} = 0.011351897$$

The reason of the spacing for the dimension of the channel supplies a constant of ratio of the mesh the variation of the diameter of the channel.

$$\frac{0,1}{0,011351897} = 8,8091$$

For the variations of the diameter of 1.3mm; 1.6mm and 2.0mm; the following ratios are had:

$$\frac{\Delta y}{\Delta x} = \frac{1.3mm}{88.091mm} = 0.014757466 \leftrightarrow \frac{0.13}{0.014757466} = 8.8091$$

$$\frac{\Delta y}{\Delta x} = \frac{1.6mm}{88.091mm} = 0.018163035 \leftrightarrow \frac{0.16}{0.018163035} = 8.8091$$

$$\frac{\Delta y}{\Delta x} = \frac{2.0mm}{88.091mm} = 0.022703794 \leftrightarrow \frac{0.2}{0.022703794} = 8.8091$$

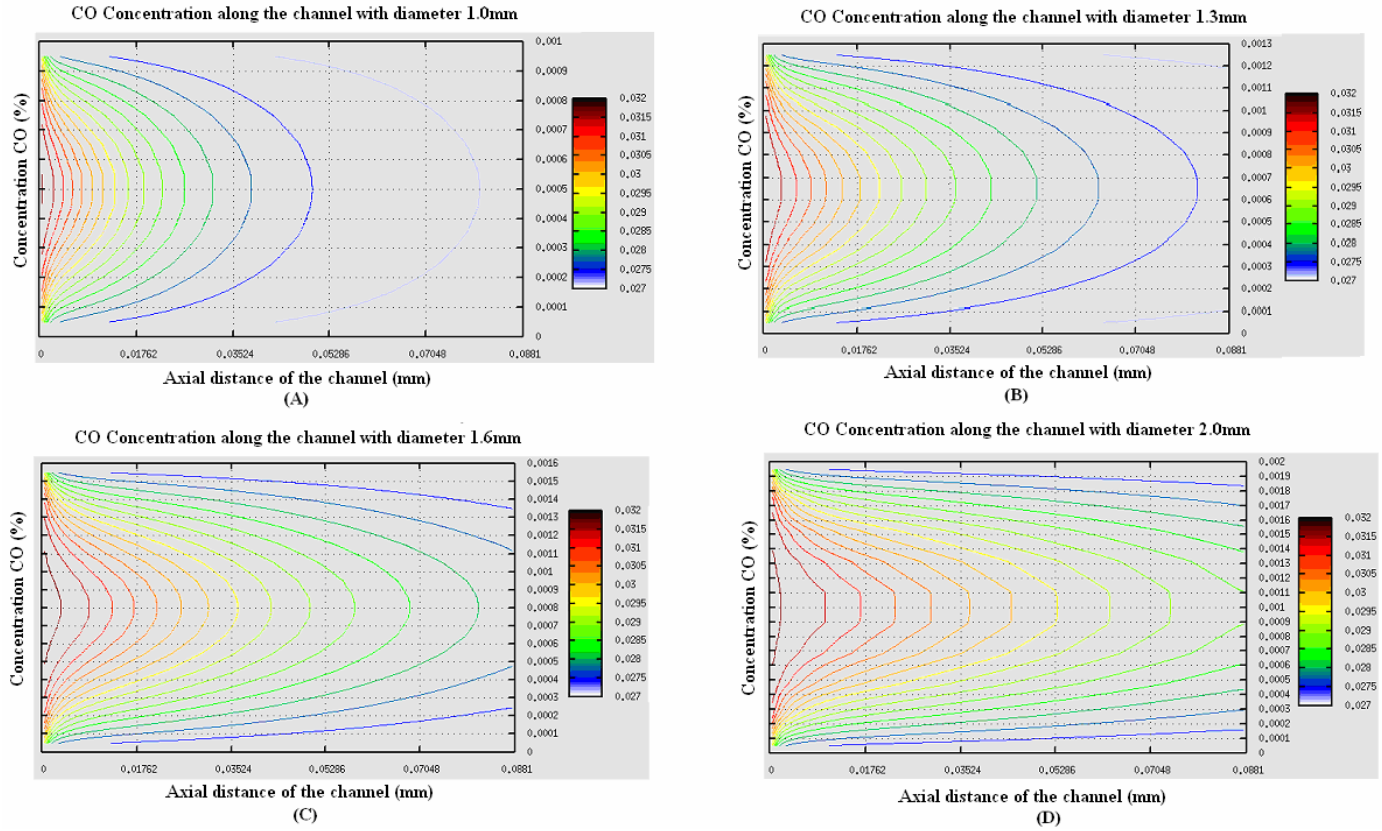

Figure 3 - The emission of carbon monoxide in the channel with changeable diameter.

The draining of the gases of exhaustion throughout a simple channel of the monolithic support and the effect of chemical reactions of catalyze are simulated by a two-dimensional model, with mesh 100x10 and first-order numerical scheme through code MFIX. The Figure 4 indicates the hydrodynamic effect and of chemical reaction of the gases burnt in transient regimen for the time t=0.01s. In this step of time, observes around the position 0.01762m of the entrance of the channel an intense process of oxidation of the concentration of carbon monoxide, this proceeding one from the diffusion and reaction in the walls of the channel, represented for the condition of contour in the wall, and this time step the gases still had exactly not reached the exit of the monolithic channel.

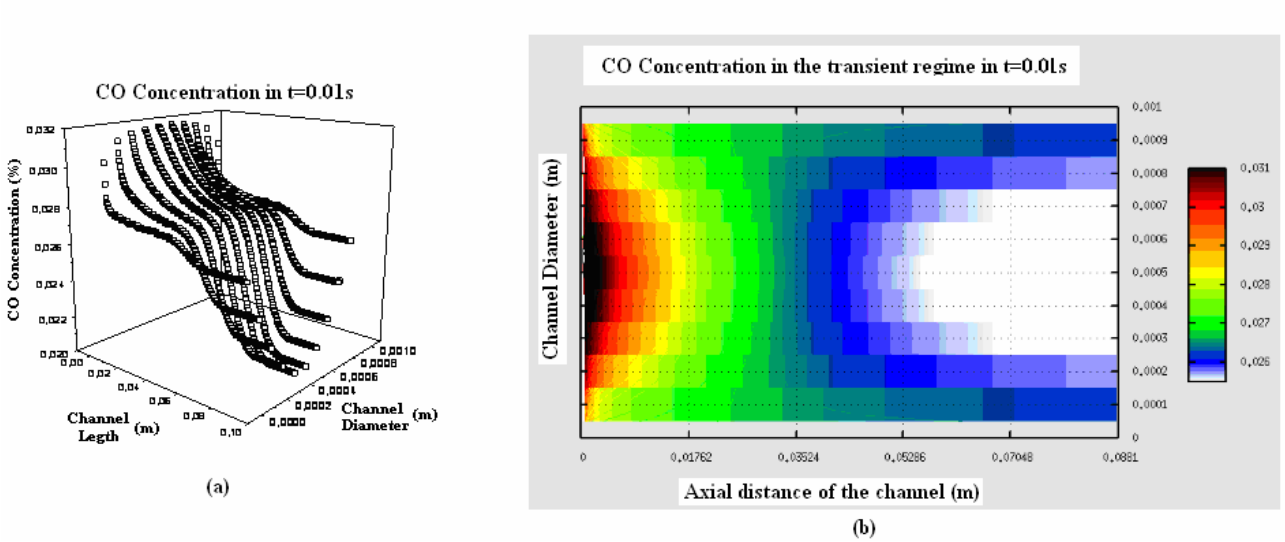

Figure 4 - The diagrams (a) and (b) represent the concentration of carbon monoxide throughout monolithic channel in the transient regimen in t=0.01seg.

The Figure 5 indicates a two-dimensional simulation gotten with code MFIX, applied the first-order numerical scheme foup, and threshes of 100x10 to long of the channel of the gases of exhaustion for the step of more advanced time t=0.2s. For this exactly time step the exhaust gases reach a regimen of draining fully developed to the long one of the channel. The species of carbon monoxide simulated in the exit of the channel was of 0.027.

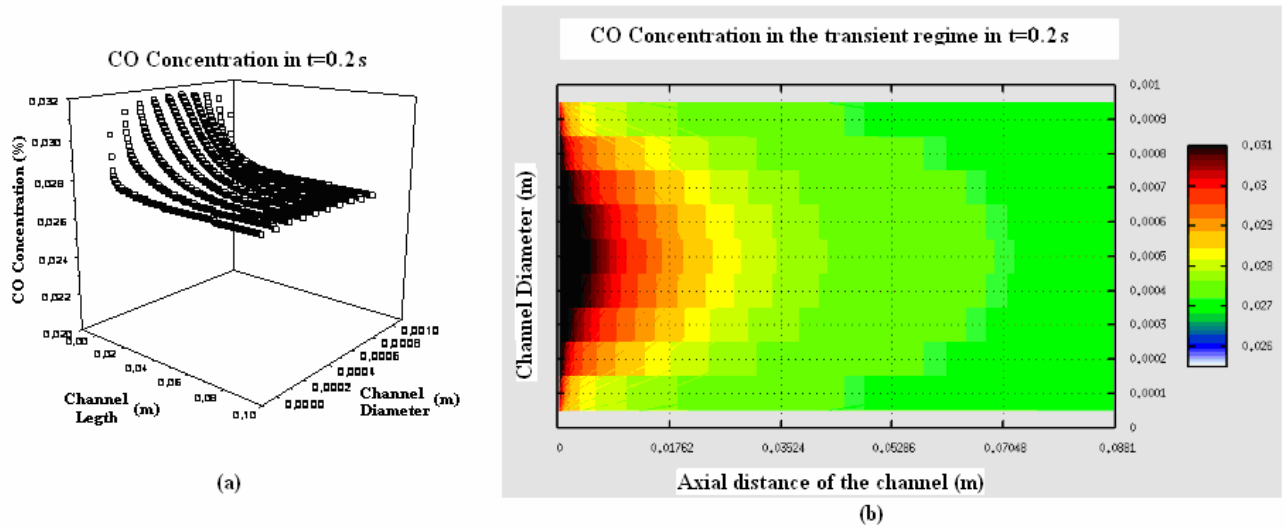

Figure 5 – The diagrams (a) and (b) represent the concentration of carbon monoxide throughout monolithic channel in the transient in t=0.2seg.

The presented results of the simulation in the fig. 6, fig. 7 and fig. 8 indicate periods of training of the solution of the equation of two-dimensional species in a simple monolithic channel, showing the process of oxidation of the concentration of monoxide of carbon to long of the channel with effect of diffusion and the reaction in the walls of the channel. Of beginning, it was remained constant computational mesh in 220x10 and got excited the numerical method in the simulation for Foup, Van Leer and Superbee in the times of 0.0120s; 0.0160s and 0.0200s, were observed that the numerical project Superbee presented approach of the numerical solution better, with lesser effect of the false diffusion.

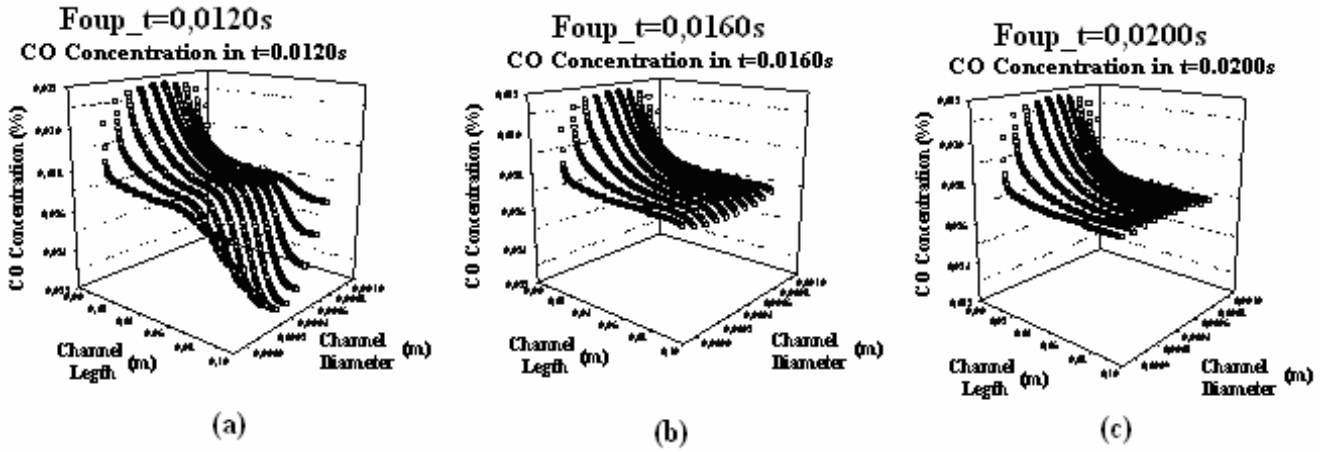

Figure 6 - Three periods of training of the solution of the equation of the two-dimensional species in a simple monolithic channel with computational mesh of 220x10 that it shows the catalysis in the process of oxidation of the concentration of carbon monoxide.

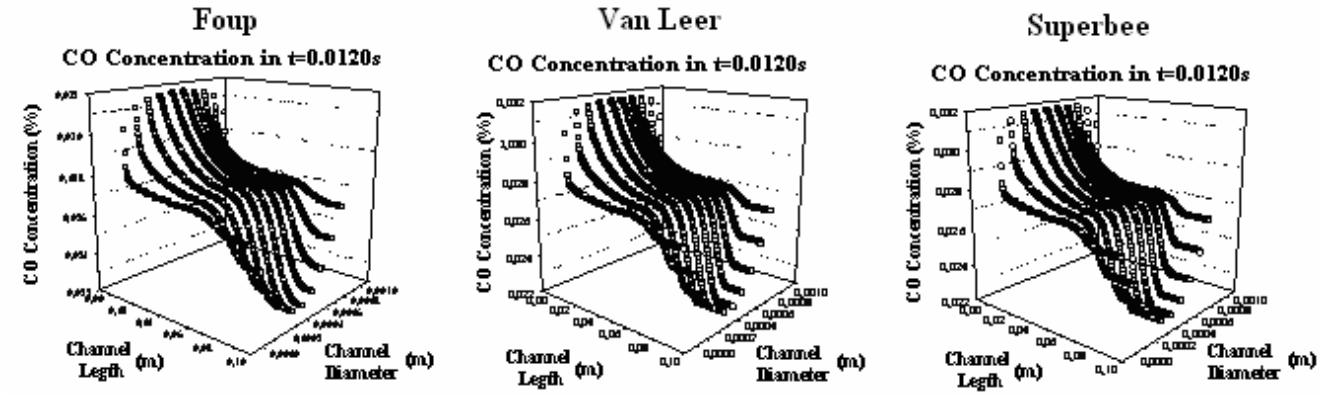

Figure 7 – Two-dimensional numerical simulation of a simple monolithic channel with mesh of 220x10, gotten with code MFIX, shows the effect of oxidation of the carbon monoxide in three different numerical scheme: Foup, Van Leer and Superbee; in the times of 0.0120s; 0.0160s and 0.0200s.

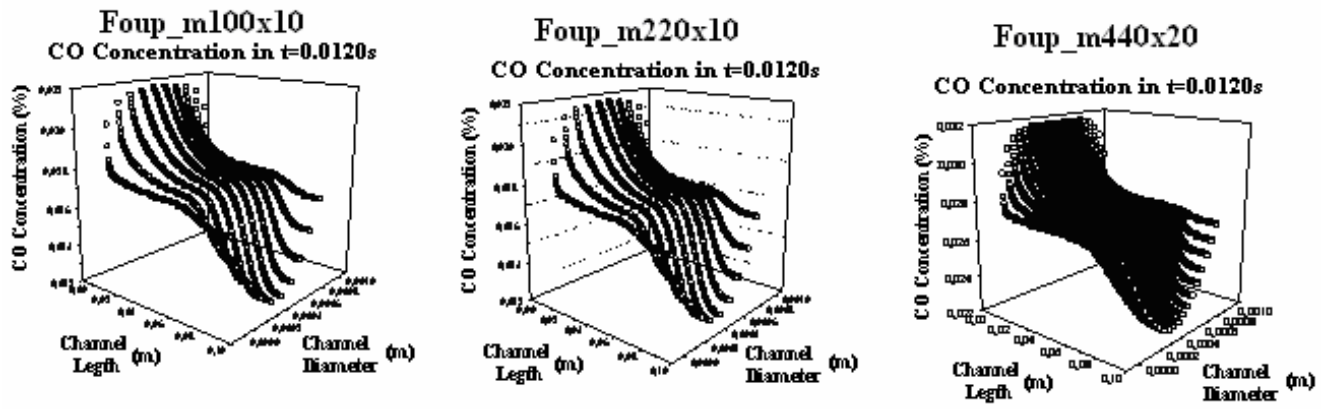

Figure 8 – Two-dimensional numerical simulation of a simple monolithic channel with first-order numerical scheme of the Foup type shows the effect of oxidation of the carbon monoxide in three different meshes: 100x10, 220x10 and 440x20 in the times of 0.0120s; 0.0160s and 0.0200s

The Figure 9 and Figure 10 indicate a comparison between the numerical scheme Foup and Superbee in the meshes thick 100x10 and average 220x10, was observed that in the numerical solution with thick mesh, first-order the Foup

scheme was turned aside from the numerical solution of the Superbee type of second order, for presenting greater numerical diffusion, while the scheme with average mesh had presented similar behavior, therefore the refining of the mesh allowed that the numerical solution of the two scheme approached more to the accurate solution.

The refinement of the mesh has as objective to observe the behavior of the solution with the space refining, making possible bigger approach of the accurate solution. The Figure 11 illustrates the refinement of the mesh of the monolithic channel for first order numerical project, Foup. The mesh 440x20 computational cells presented a solution that converged to a solution that are next to the accurate solution with and minor numerical diffusion in relation to the other meshes 100x10 and 220x10. According to Maliska (1995) the numerical diffusion diminishes with the refining of the mesh and the numerical solution if it approaches to the accurate solution.

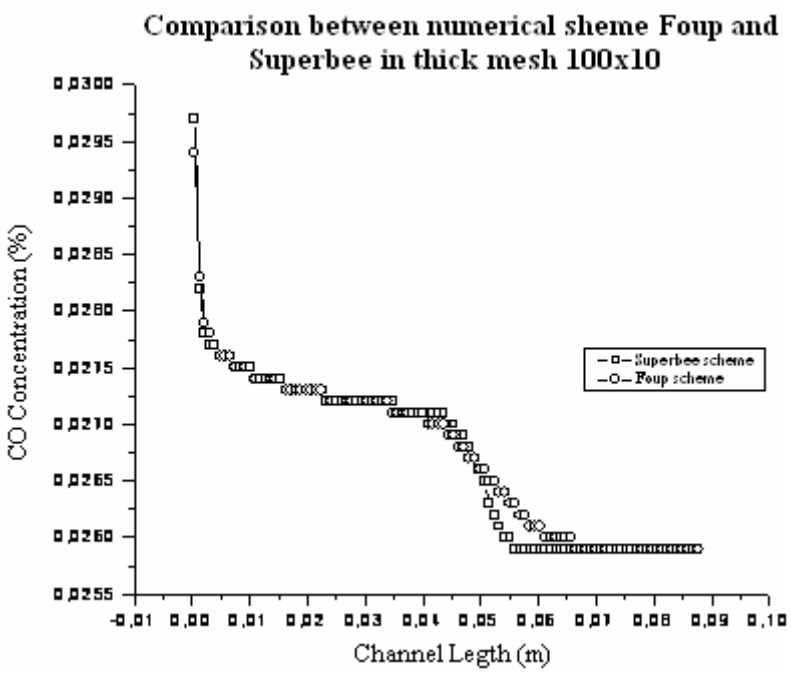

Figure 9 - Comparison between the numerical scheme Foup and Superbee in the thick mesh 100x10.

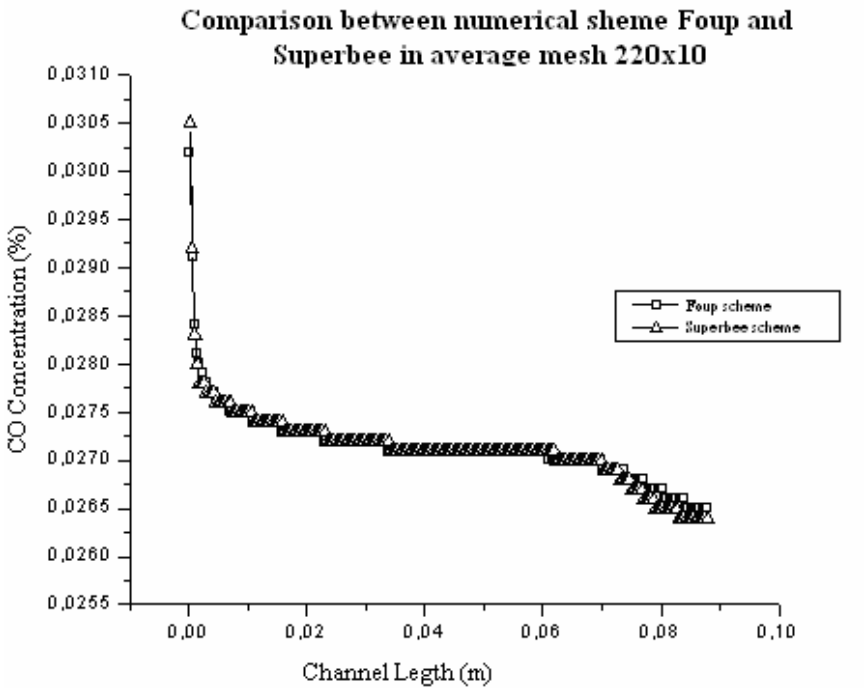

Figure 10 – Comparison between numerical scheme Foup and Superbee in the average mesh 220x10.

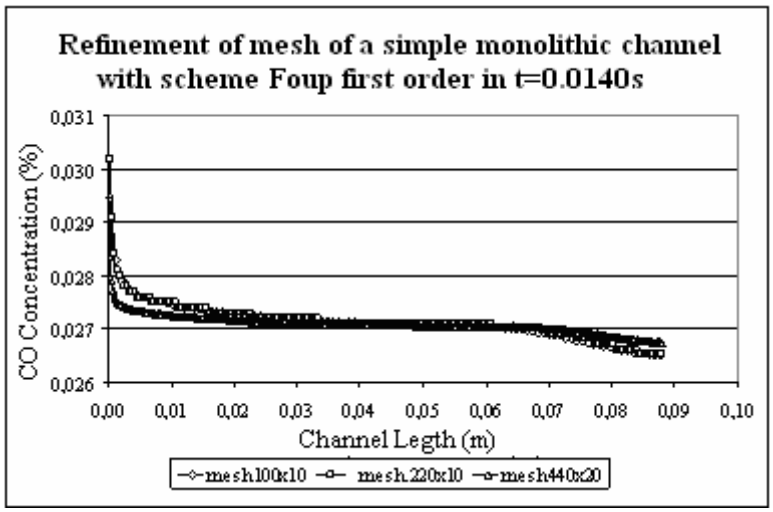

Figure 11 - Refinement of mesh of a simple channel of the monolithic

6. Conclusions

The hydraulical diameter of the monolithic channel was increased gradual of 1mm 2mm, verified an esteem loss of 7.4% of the catalytic efficiency.

It was evidenced that the refinement of the mesh in the monolithic channel allowed a numerical solution with reduced effect of numerical diffusion, independent of the used numerical scheme, however the processing time increased in too much.

The curves of carbon monoxide had presented fellow creature behavior with application of the numerical scheme foup and superbee in the average mesh, what it favors the use of a thicker mesh with scheme of second order diminishing the time of processing of the PC.

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9. Responsibility notice

The authors are the only responsible for the printed material included in this paper.