DYNAMIC SIMULATION OF A COLLECTOR OF H_2 USING A DYNAMIC LIBRARY

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ABSTRACT
This work treats the problem of dynamic simulation of a collector of H_2 in a refinery, as the first step for the development of a dynamic simulation of the complete network of H_2. There try to be studied the phenomena of transport of matter and energy of the collectors of H_2 from the point of view of the pressure, temperature, molecular weight, etc., having in it counts the spatial distribution of the same ones. For it, we use a graphical library developed in EcosimPro® that allows the study of different structures.

Keywords: dynamic simulation, networks of hydrogen, numerical methods, dynamic library of components in EcosimPro®.

1. INTRODUCTION

The present work allows to a wider project of investigation. Its aim is of developing new knowledge in the field of the control and systems optimization of large scale in the process industry and demonstrating his applicability on an industrial scale.

The interest for this type of systems has been growing progressively for his impact in the global functioning of a system or factory, so much economically as technician, as for the strategic paper that often they recover (Prada 2004). Between them they find the distribution networks: of water, of electricity, of gas, of telecommunications, etc., of whose effective management there can depending both the satisfaction of the demands of the users and the profitability of his operation. Especially, the networks of steam distribution, gas, water treatment, etc. of many industries of processes they connect the centers of production or storage with the plants where the above mentioned resources are consumed across a distribution system which habitual characteristics are his large scale, the interaction between the different elements, the variability of the demands, the presence of diverse restrictions of operation and the control of his functioning across decisions of different nature. The production of hydrogen in large quantities today is only feasible from hydrocarbons in plants where the principal element are the ovens of reformed. From them it is distributed to the different consuming plants across a complex system of pipelines (collectors) of several kilometers of length, different diameters and working to different pressures and purities.

Though the networks have several kilometers along a refinery, his capacity of storage is very limited, for what to guarantee the fulfillment of the changeable demands of the consuming plants an excess of hydrogen is kept in the distribution network that ends up by being sent to the gas network to fuel consumption in ovens and other equipments mixed with other fuels or, eventually, to the torch of the refinery. However, to the being the hydrogen an expensive gas of producing, is not desirable an overproduction though this one assures the supply of the consuming plants. On the other hand a fault of hydrogen can limit the production or the life of the catalysts of the reactors. For it, the management of the network must attend simultaneously to a level of control of pressures and flows of the system and to a level of optimization of the global decisions. The topic of the optimization has been approached by means of an approach based on the determination of the condition of the network and on the next optimization of the decisions, on the frame of a system of help to the capture of decisions (Gómez et al. 2008) and (Sarabia et al. 2009). The above mentioned approach is based in addition on stationary models of the network of H_2, supposing that the flow is a ideal gas mixtures and without bearing in mind the spatial distribution of the own network. However, since normally the control system of the network is decentralized, with classical control structures, may not be easy to implement the global recommendations of the optimizer for whole network both the interactions between its components as dynamics constraints of low level of flows and pressures that have not been taken into account explicitly to level of optimization.

2. DESCRIPTION OF THE COLLECTOR OF H_2

To know the dynamics of the variables (density, pressure and temperature) in function so much time as of the longitudinal coordinate of the conduction, appear the corresponding balance sheets of mass, quantity of movement and energy based on a macroscopic description. In addition it is supposed that in the direction of the radial coordinate there is no variation of

density, pressure and temperature, that is to say, the model goes global with regard to this coordinate. Next there appear the equations of the model distributed of the collector. The equation (1) describes the global mass balance when the phenomenon of transport is only due to the convention (Ames 1977):

$$\frac{\partial m}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(rv_r m)+\frac{1}{r}\frac{\partial}{\partial \theta}(v_\theta m)+\frac{\partial}{\partial z}(v_z m) = \frac{1}{r}\frac{\partial}{\partial r}\left[\rho \widetilde{D}_R r\frac{\partial}{\partial r}\left(\frac{m}{\rho}\right)\right]+\frac{1}{r^2}\frac{\partial}{\partial \theta}\left[\rho \widetilde{D}_\theta \frac{\partial}{\partial \theta}\left(\frac{m}{\rho}\right)\right] + \frac{\partial}{\partial z}\left[\rho \widetilde{D}_z \frac{\partial}{\partial z}\left(\frac{m}{\rho}\right)\right]+R \quad (1)$$

Being variables m, v_r, v_θ, v_z, ρ, $\widetilde{D}_R$, $\widetilde{D}_\theta$, $\widetilde{D}_z$, r, θ, z y t are the mass, component of the speed in direction *r*, component of the speed in direction θ, component of the speed in direction *z*, density of the fluid, component of the coefficient of dispersion in direction *r*, component of the coefficient of dispersion in directionθ, component of the coefficient of dispersion in direction *z*, radial coordinate, angular coordinate, longitudinal coordinate and time, respectively. The equations (2) and (3) show the individual mass balance being C_k is the composition of the component k (hydrogen and impurities):

$$\frac{\partial(mC_k)}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(rv_r mC_k)+\frac{1}{r}\frac{\partial}{\partial \theta}(v_\theta mC_k)+\frac{\partial}{\partial z}(v_z mC_k) = \frac{1}{r}\frac{\partial}{\partial r}\left[\rho \widetilde{D}_R r\frac{\partial}{\partial r}\left(\frac{mC_k}{\rho}\right)\right]+\frac{1}{r^2}\frac{\partial}{\partial \theta}\left[\rho \widetilde{D}_\theta \frac{\partial}{\partial \theta}\left(\frac{mC_k}{\rho}\right)\right] + \frac{\partial}{\partial z}\left[\rho \widetilde{D}_z \frac{\partial}{\partial z}\left(\frac{mC_k}{\rho}\right)\right]+R \quad (2)$$

$$\sum C_k = 1 \quad (3)$$

The equation (4) shows the quantity of movement balance:

$$m\left(\frac{\partial v_z}{\partial t}+v_r\frac{\partial v_z}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}+v_z\frac{\partial v_z}{\partial z}\right) = -\frac{\partial P}{\partial z}Vol + \left[\frac{1}{r}\frac{\partial}{\partial r}\left(\tilde{\mu}_{zr} r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\frac{\partial}{\partial \theta}\left(\tilde{\mu}_{z\theta}\frac{\partial v_z}{\partial \theta}\right) + \frac{\partial}{\partial z}\left(\tilde{\mu}_{zz}\frac{\partial v_z}{\partial z}\right)\right]+mg_z \quad (4)$$

Being P, $\tilde{\mu}_{zr}$, $\tilde{\mu}_{z\theta}$ y $\tilde{\mu}_{zz}$ correspond with the pressure of the fluid and with the effective viscosity in coordinate *r*, θ y *z*, respectively. It thinks that the fluid that circulates along the interior of the pipeline suffers loss of quantity of movement due to the friction. Then, this term is added in the second member of the equation (4): $P_{roz} = -\rho\frac{\emptyset}{2d}v\|v\|$. Equation (5) shows the corresponding energy balance, where there has not been included the phenomenon of the viscous dissipation that is the conversion of the kinetic energy in heat owed to the internal friction to the fluid since it is possible to consider it despicable.

$$mC_p\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+\frac{v_\theta}{r}\frac{\partial T}{\partial \theta}+v_z\frac{\partial T}{\partial z}\right) = \frac{1}{r}\frac{\partial}{\partial r}\left(\tilde{k}_R r\frac{\partial T}{\partial r}\right)+\frac{1}{r^2}\frac{\partial}{\partial \theta}\left(\tilde{k}_\theta\frac{\partial T}{\partial \theta}\right)+\frac{\partial}{\partial z}\left(\tilde{k}_z\frac{\partial T}{\partial z}\right) + S_R \quad (5)$$

Being C_p, T, $\tilde{k}_R$, $\tilde{k}_\theta$ y $\tilde{k}_z$, are it respectively the calorific capacity, the temperature and the component of the conduction in the coordinates *r*, θ y *z*. It thinks that along the pipeline heat losses exist towards the exterior. This term gets in the second member of the equation (5): $Q_{pérdidas} = -U(T-T_{ext})$, being U the global coefficient of heat transmission. Finally, there is had the equation of the ideal gases since the gas that circulates along the interior of the collectors is not to very high pressures and temperatures:

$$PV = nRT \quad (6)$$

Being V the volume, n the number of masses and R the constant of the ideal gases.

3. MODELLING IF THE COLLECTOR OF H_2

The analytical approximation methods of the solution of an equation in partial derivatives, provide frequently useful information over of the behavior of the solution in critical values of the dependent variable, but they tend to be more difficult to apply that the numerical methods (González 2008). The numerical methods are technical by means of which it is possible to formulate mathematical problems in such a way that they could be solved using arithmetical operations. The use of distributed models for (1) - (6) exclude the utilization of conventional integrators to integrate the model. The collocation orthogonal method and finite differences method are widely used to solve numerically equations in derivatives partial (PDEs), transforming the partial derivatives into a set of differential ordinary equations (ODEs) doing a discretization the spatial domain.

3.1. Finite Differences

The finite differences method is widely used to solve numerically equations in derivatives partial (PDEs), transforming the partial derivatives for an approximation into a set of differential ordinary equations (ODEs) doing a discretization the spatial domain. In this method, a derivative equation in a discreet point, x_j, is evaluated using the information about the variables in this point x_j (local information). One of the big advantages of the finite differences method is the wealth of existing theory to help solve different problems. Topics like the numerical consistency, convergence and stability have been deeply studied. In addition it offers a considerable flexibility

when one works in discretización of meshes since there can be chosen the dimensions of time and space and it is a question of a method intuitive and easy to help. There are several variations on the finite differences method and they are function of how to perform the approach of the partial differential equation (Ramírez et al. 2006). However, the finite central difference is often the most exact and it is the used one in this work.

3.2. Collocation orthogonal

The collocation orthogonal method is a variant of the method of weighted residues, where the nodes of approximation are given by the roots of orthogonal polynomials as those of Jacobi, Legendre and Hermite, between others. The polynomial approximation is done in the whole domain. This methodology offers major precision those other methods, since the equation of discretización for a node involves to all the nodes of the domain. The choice of these collocation points remains of some arbitrary form until there appears the work (Villadsen and Stewart 1967), those who establish the choice of the collocation points as the roots of orthogonal appropriate polynomials. There exist some variants that depend in the form of the function of test and in the form of selecting the location of the nodes, as: simple collocation with function Dirac's Delta, Sub-domains, Moments, Galerkin, Square Minimums, etc. (Finlayson 1980), (Ames 1977).

3.3. Collocation orthogonal on finite elements

In the finite elements method, the domain is subdivided into a set number of small regions, where each is unique. On each finite element, the dependent variables (temperature, speed, concentration, etc.), are approximated by using known functions. These functions can be linear or nonlinear (polynomials generally), depending on the nodes used to define finite elements. Next, the model equations are integrated in each finite element and the set of individual solutions that are obtained are assembled on the total domain. As consequence of these operations, one obtains a set of algebraic equations which is solved for know the value of the dependent variables in the nodes (Finlayson 1980). This method is suitable for problems with irregular geometries. Next, the finite elements are coupled following the principle of continuity. This methodology is adapted for problems in those who are known that abrupt changes exist in the values of the dependent variables (Carey and Finlayson 1975).

3.4. Finite Volumes

It is considered to be a discretization mesh of the fluid space. Around each point of this grid is built a control volume that does not overlap with those of neighboring points. Of this form, the total volume of fluid will have to be equal to the sum of the considered control volumes. The set of differential equations for a model is integrated over each control volume, which translates as a discretization of the set of equations. The finite volume methods are narrowly related to the finite differences methods (Leveque 2004). It is intuitive to think that the accuracy will be greater the lower the volume size; by what is interesting divide the domain into as many pieces as possible. The price to pay is that the coefficient matrix of the system to be solved is large, so the computational cost of resolution can be increased greatly if the number of nodes is too high. The point of commitment is reached when it find the mesh with the minor possible number of nodes that there provides a solution independent from this one, that is to say, a mesh in which the solution does not change significantly if the space reduces.

4. LIBRARY OF COMPONENTS IN ECOSIMPRO FOR DISTRIBUTED SYSTEMS

Creating a dynamic library of components (Figure 2) in EcosimPro® allows constructing of simple form different models. The components of "*Entrada*", "*Salida*", "*Aporte*", "*Consumo*" and "*Tubería*" contain the described equations of (1) - (6) discrete using the numerical methods. The components "*Nodo_1a2*" and "*Nodo_2a1*" contain equations of continuity.

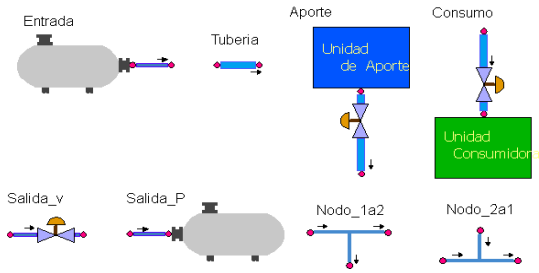

Figure 1: Librería de componentes en EcosimPro®

The component of "*Entrada*" comes from a warehouse, so the contour conditions in this point will be the pressure, the temperature and the concentration of the fluid. The component "*Aporte*" has a valve in the beginning of the pipeline, for what the velocity, the temperature and the concentration of the fluid is boundary conditions. On the other hand, the component "*Consumo*" finishes with a valve that will be at the entry of the consuming units and, for this reason, in this point the velocity is a boundary condition. Finally, analyzing the component "*Salida*", it is possible to have at the end of the pipeline a valve or a warehouse. Then, the boundaries are the velocity or the pressure, respectively. Depending of the bounds of boundaries that are chosen, the problem to resolving is different. To bear it in mind different components have been included. With this library of components can be realized precise analyses of transitory. In addition, he presents the advantage of which it is possible to extend of rapid and simple form with new components that could turn out to be necessary for the simulation of the most complex systems, for example, components of type of control as regulators PID, etc.

5. EXAMPLE AND RESULTS

The example consists into considered the system of the Figure 2, which it has a collector formed by two units of

contribution and three consuming units. The Table 1 shows the number of equations, the number of variables and the time that is late the simulation in executing 600 seconds. In the Table 2 there appears the number of nodes in which every component has been divided. The difference in simulation time is due to the type and number of equations that are used. The collocation orthogonal method in finite elements has the greatest number of equations and variables (since it has more nodes) and it has the bigger simulation time.

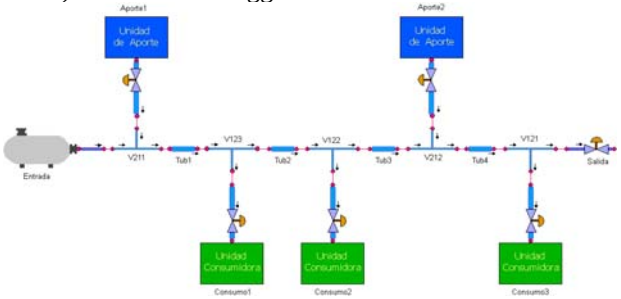

Figure 2: Example of a collector with two units of contribution and three consuming units

Table 1: Number of equations and variables

	CO	CO in EF	DF	VF
Nº eq.	929	1406	1397	807
Nº var.	1369	1720	1864	1101
Simulation time (s)	2.953	4.828	3.640	2.578

Table 2: Number of nodes of every component

	CO	CO in EF	DF	VF
Nº Nodes Interiors	2	2	5	5
Nº Nodes Total	N_{tot}=4	Nº EF: 2 N_{tot} = 7	N_{tot}=7	N_{tot}=7

It has been realized a jump in the composition of the fluid of entry to the collector that proceeded from the component "*Entrada*" to see the evolution of the composition of the fluid along the collector. At first, all the compositions of contribution are equal (purity of the hydrogen of the 99.9 %). Next, the composition of "*Entrada*" happens to be 99.85 % in purity of the hydrogen. To see clearly the results, it is represented in the graphs the first node of every component of the principal collector (it is to say, the first nodes of the components "*Entrada*", "*Tubería*" y "*Salida*").

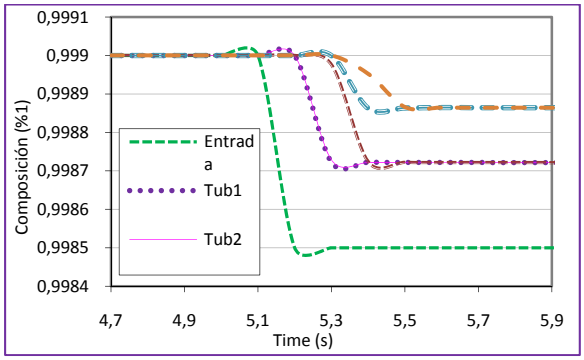

Figure 3: Composition of the collector using CO on having changed the composition of "*Entrada*"

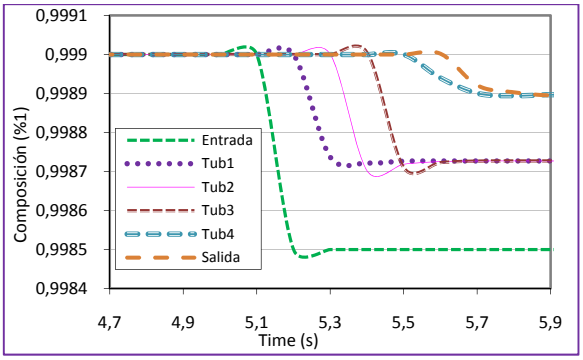

Figure 4: Composition of the collector using CO in EF on having changed the composition of " *Entrada*"

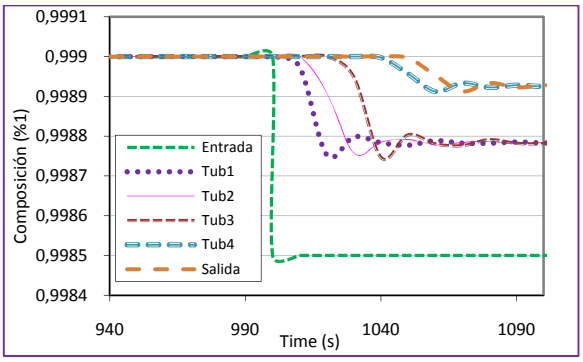

Figure 5: Composition of the collector using DF on having changed the composition of " *Entrada*"

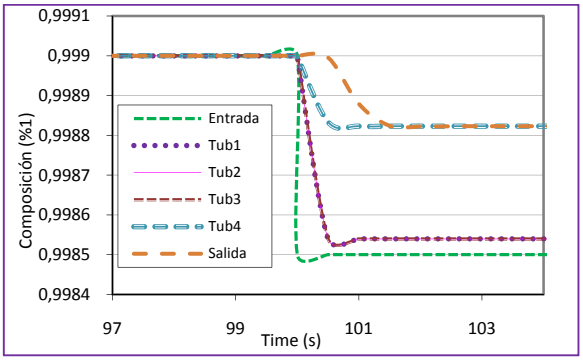

Figure 6: Composition of the collector using VF on having changed the composition of " *Entrada*"

As show the figures 4 - 7, on having diminished the composition of the fluid of entry to the principal collector, it diminishes the composition along the collector since this variation is transmitted from a component to other one. It is necessary to emphasize that the composition of the components "*Tubería1*", "*Tubería2*" and "*Tubería3*" is same, but different from the composition of "*Entry*" since in the middle exists a current of contribution, "*Aporte1*" whose fluid possesses a composition of 99.9 % in purity of H_2. The same thing happens with the composition of the components "*Tubería2*" and "*Exit*", that though between them they have the same composition, this one is different from the rest of the components of the principal collector since in this point appears a new current: "*Aporte2*" with a 99.9 % in purity of H_2. Also it is possible to observe that the response of the model before these changes is soft, of the second order,

underdamped and with a small time of stabilization (except for the case of finite differences). As expected, there is a delay in the response of the fluid as it moves through the collector. Next a jump is done in the composition of entry to the principal collector from the component *Aporte1*" happening from 99.9 % to 99.86 % and after 99.86 % to 99.91 %.

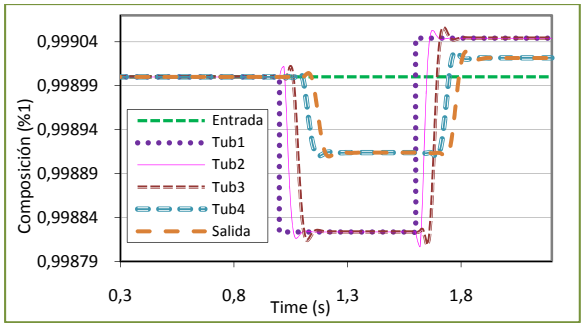

Figure 7: Composition of the collector using CO on having changed the composition of "*Aporte1*"

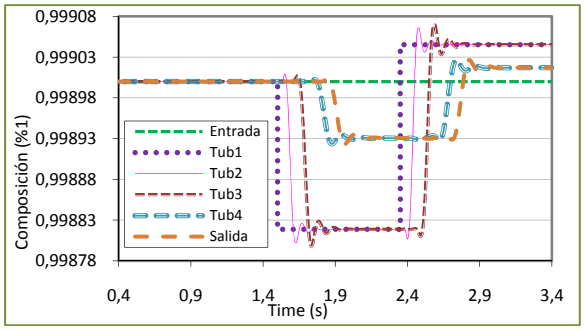

Figure 8: Composition of the collector using CO in EF on having changed the composition of "*Aporte1*"

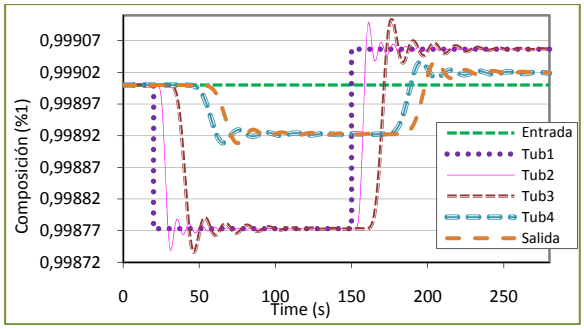

Figure 9: Composition of the collector using DF on having changed the composition of "*Aporte1*"

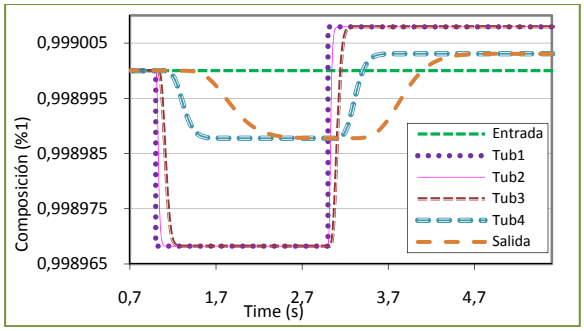

Figure 10: Composition of the collector using VF on having changed the composition of "*Aporte1*"

In this case, the composition of the fluid in the component "Entrada" does not intervene since the component "Aporte1" appears in a place later, so this composition always will have the same value. The conclusions obtained are equivalent to those of the previous case as for the type of response that is obtained and to the value of the composition along the collector. Another type of jump that has been realized is the change in the pressure of entry to the collector from the component "Entrada". Initially, the pressure of entry to the collector is of 1.8982 • 106 Pa (18.7 atm.) and later there happens to cost 1.8907 • 106 Pa (18.6 atm.).

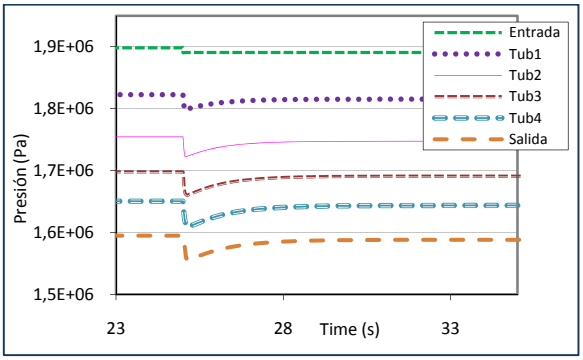

Figure 11: Pressure of the collector using CO on having changed the pressure of "*Entrada*"

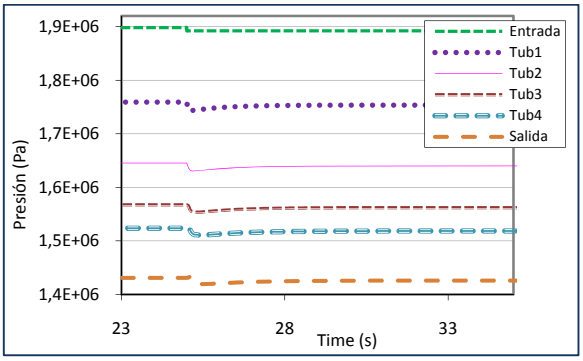

Figure 12: Pressure of the collector using CO in EF on having changed the pressure of " *Entrada*"

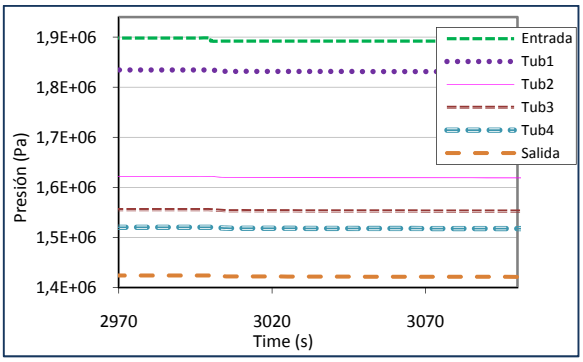

Figure 13: Pressure of the collector using DF on having changed the pressure of " *Entrada*"

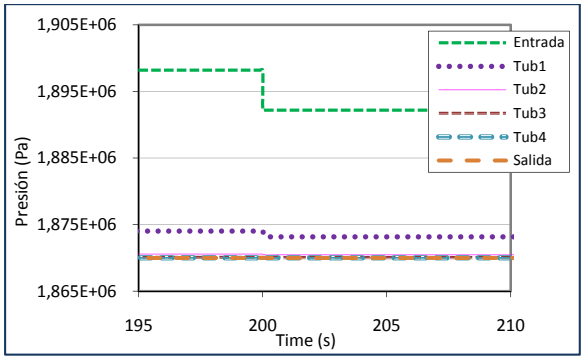

Figure 14: Pressure of the collector using VF on having changed the pressure of " *Entrada*"

As shown in Figures 12-15, a decrease in inlet pressure causes a decrease of the pressure along the collector. In the case of orthogonal collocation and orthogonal collocation on finite elements, the kind of response you get is underdamped, the response in every case has a small stabilization time. Also we can found significant changes in the density of the fluid since that increasing pressure increases the mass and, for a constant volume, density increases, and vice versa. The other variables also change, but its effect is not so obvious.

6 CONCLUSIONS

There has been created a graphical library of dynamic components that allows to constructing of easy form complex systems of pipelines. Of this form, it is possible to study the dynamics of a fluid that circulates in different systems. It is a question of a very useful tool that in a future work will be extended with components of control.

The results obtained in the simulations are coherent with the physical and chemical laws formulated.

In the simulation, obstacles were encountered at the moment of the initialization of the problem, but these are resolved of satisfactory form. However, one is working in order that the resolution of these problems of initialization is realized of automatic form.

Finally, we have found many bibliographical references that explain the fundaments of the methods of integration. Generally they use the example of a bar that warms up in an end and they apply these methods to solve the equation of heat conduction. Others use the equation of movement in examples like porous beds, catalytic beds, etc. However, we have not found enough references that combine the equations of conservation of mass, conservation of movement and heat conduction, which are those who are used in this work.

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