

A Taylor-Galerkin method for the use of finite elements in a nonlinear problem for the numerical modeling of a new Chemo-Fluid oscillator

Illych Álvarez¹, David Terán², Danny Dessechis³.

¹ Facultad de Ciencias Naturales y Matemáticas, Escuela Superior Politécnica del Litoral, Km. 30.5 Vía Perimetral, Guayaquil, Ecuador

ialvarez@espol.edu.ec

² Facultad de Ciencias Naturales y Matemáticas, Escuela Superior Politécnica del Litoral, Km. 30.5 Vía Perimetral, Guayaquil, Ecuador

davetera@espol.edu.ec

³ Facultad de Ciencias Naturales y Matemáticas, Escuela Superior Politécnica del Litoral, Km. 30.5 Vía Perimetral, Guayaquil, Ecuador

dany@espol.edu.ec

ABSTRACT

In this work, a finite element scheme is proposed using a method of Euler-Taylor-Galerkin described in Páez (2016), for a non-linear model which describes the behavior of a new chemo-fluidic oscillator (Donea, 1984). This model is expressed by the coupling of an ordinary differential equation describing the hydrogel dynamics, the non-linear transport equation and an auxiliary equation determining the flux volume. The numerical solution is constructed by taking a semi-discretization in time of the transport equation, employing forward-time Taylor series expansions including time derivatives of second order and third order, avoiding instabilities problems. In this semi discrete equation, the spatial variable is approximated by the finite element formulation according to Galerkin. Some simulations are carried out taking different initial conditions for the concentration of the hydrogel. The numerical results describe the oscillatory behavior of the system as in Donea (1984), where MatLab tools are used as black box.

Keywords: [New chemo-fluidic oscillator], [Non-linear model],[Finite element], [hydrogel dynamics].

Introduction

Self-oscillating systems play an important role in both the natural sciences (biology or chemistry) and technology (micro electromechanical or electronic systems) because they can be coupled to other

systems; one of their most important applications is the use as a system clock to trigger regular events such as circadian rhythm or in electronic systems.

This work refers to the use of a Taylor-Galerkin method for applying finite element to the nonlinear system that controls the behavior of the new chemo oscillator-fluidic and determine its numerical modeling. The mathematical problem was raised by Páez[1]who made a numerical approximation of the transport PDE using the well-known Line Method, however, the ODEs system provides a very rough approximation of the solution of the transport equation.

First, this is due to the first-order discretization in space and secondly because it can propagate abrupt changes or steep fronts, which is a well-known computational problem in the numerical solution of hyperbolic PDE.

In order to describe the dynamics of the chemo-fluidic oscillator a set of mathematical models was used, which posed a challenge due to the complexity of the system, since the oscillator is affected by various nonlinearities that come from the characteristics of the hydrogel and the bidirectional coupling between the chemical and fluidic domains. The hydrogel is designed in such a way that an increase in the concentration of alcohol reduces its size and vice versa. Therefore, at low concentrations of alcohol, the hydrogel valve is closed, while high concentrations of alcohol open the valve. A bypass channel is connected to the valve inlet, to allow a continuous flow of unidirectional fluid near the hydrogel independent of whether the hydrogel valve is open or closed.

Therefore, to facilitate the modeling process, the system was divided into the fluidic domain describing the behavior of volumetric flows and system pressures during the operation and chemical domain which in turn divided into two parts the description of hydrogel dynamics and the modeling of the delay line, resulting in a coupled system composed of the one-dimensional transport PDE, the ODE that models the dynamic behavior of the hydrogel and the equation that determines the volume in the buffer.

To perform this work following very closely to what Donea [2]did, the equation is semi-discretized of nonlinear transport using Taylor's serial expansions at the time of first, second and third order to obtain a second order differential equation in the space in which we apply Galerkin's variational formulation to use the finite element method and obtain the system of linear equations that needs the value of the variable that determines the size of the hydrogel that is obtained for each instant of time by applying the Runge -Kutta 4 method and the buffer volume that is found using numerical integration methods.

Analyzing in more detail its mathematical modeling and the numerical solution of this New Chemical-Fluidic Oscillator based on intelligent hydrogels was one of the reasons for the realization of this work in addition to extending the linear method used by Donea [2] for the nonlinear transport equation and providing a solution methodology for models of new oscillators involving the nonlinear one-dimensional transport equation.

1.Design of a chemo-fluoscillator

The new fluidchemo oscillator is based on a negative feedback circuit containing a delay line, where negative feedback is provided by a hydrogel valve that has the ability to change its size depending on the temperature and concentration of the aqueous solution that is in direct contact with the hydrogel. In this new oscillator the temperature remains constant so the only parameter that produces a change in the size of the hydrogel is the concentration of alcohol.

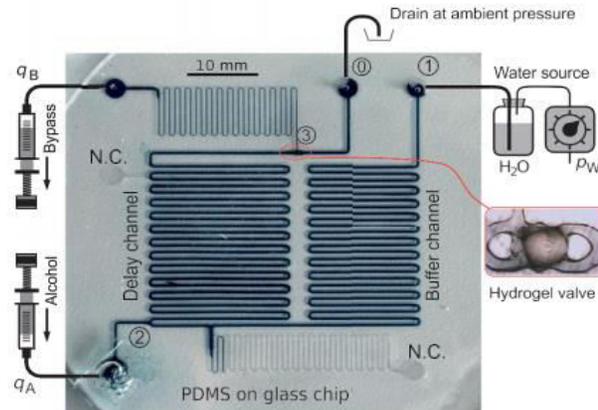


Figure 1. Photography of the manufactured chemo-fluidic oscillator circuit, filled with a highly dyed solution for better visibility of the channels. External sources of constant flow and pressure are shown schematically. Equivalent fluidic circuit. The hydrogel valve is represented by a controlled flow source.

The oscillator is powered by three constant sources. The first is a constant flow source q_A that supplies the system with an alcohol concentration solution c_{alc} . A second source provides deionized water at a constant pressure p_W located at Node 1. Water flows through a long channel called the damping line and then is mixed into Node 2 with the alcohol solution provided by q_A , and then the mixed solution enters the channel of the long fluid that acts as a delay line. Using this channel, the solution is transported at a rate determined by the flow through the delay line $q_2(t)$ and its cross-section. The end of this channel is connected to the inlet of the hydrogel valve, whose fluid behavior is controlled by the alcohol concentration of the solution. Finally, a bypass channel connects to Node 3 to drain the liquid to a conveniently chosen constant flow rate q_B .

The micro-fluid system will be modeled through Kirchhoff's laws, within the framework of network theory for a circuit. This approach is used by how small the dimensions of the magnitudes that govern the operation of the oscillator within the study of the micro fluids since they are in a range of micronano and picoliter, therefore, the pressure is considered analogous to the voltage and volumetric flow rate to the electric current, as well as the lines of delay to the resistors. In this context, the oscillator can be described by the fluid network presented in Figure 2.

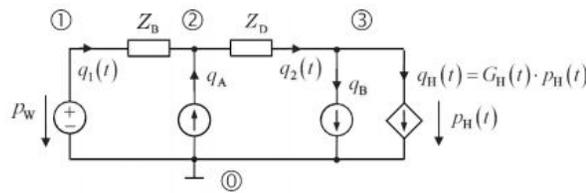


Figure 2. Equivalent fluidic circuit. The hydrogel valve is represented by a controlled flow source.

2.Mathematical model of chemical oscillator-fluidic

The mathematical problem to be studied was raised by Páez et al. in [1], and consists in finding functions $l_v: [0, T] \times [0,1] \rightarrow R_+$ such that:

$$\frac{dl_v}{dt}(t) = \gamma[C(t, 1)]\{l_{eq}[C(t, 1) - l_v(t)] \Rightarrow \begin{matrix} l_v^0, C^0(x) = C_{ini}(x) \quad \forall x \in (0, 1] \\ l_v^{n+1} = F(l_v^n, C^n(1); \Delta t), n = 0,1,2, \dots, N \end{matrix} \quad (1)$$

$$l_v(0) = l_v^0$$

$$\begin{aligned} \frac{\partial C}{\partial t}(t, x) + v(l_v(t)) \frac{\partial C}{\partial x}(t, x) &= 0, \forall (t, x) \in (0, T] \times (0, 1]; \\ C(0, x) &= C_{ini}(x), \quad \forall x \in [0, L_d]; \\ C(t, 0) &= C_a(t), \quad \forall t \geq [0, T]; \end{aligned} \quad (2)$$

The data in this problem are the functions $Y, l_{eq}, v, C_{ini}, C_a, l_v^0$, and where $C(t, 1)$ is the unknown value to be determined from the function $C(t, x)$ at the end $x = 1$; which must also be determined simultaneously, in this problem, the function $V_{buff}(t): [0, T] \rightarrow R^+$ defined by:

$$V_{buff}(t) := \int_0^t q_2[l_v(s)] ds - q_A t; \forall t \in (0, T], \quad (3)$$

Where q_2 is a known function and q_A is a constant also known

2.1 Semi - discretization in problem time (2)

The transport equation is considered

$$\frac{\partial C}{\partial t}(t, x) = -v(l_v(t)) \frac{\partial C}{\partial x}(t, x), \forall (t, x) \in (0, T] \times (0, 1];$$

If it is denoted by $C^n(x)$ the value of the function $C(t, x)$ evaluated on the node $t = t^n$, then a schema in finite differences very simple to approximate the temporal derivative in (4) would be the one obtained by the serial expansion of Taylor, in the first order, around the point $t^{n+1} = t^n + \Delta t$:

$$C(t^n + \Delta t, x) = C(t^n + \Delta t) + \Delta t \left[\frac{\partial C}{\partial t} \right] (t, x) |_{t = t^n} + O(\Delta t)$$

From here, despising the $O(\Delta t)$ you have:

$$\left[\frac{\partial C}{\partial t} \right] (t, x) = \frac{C^{n+1}(x) - C^n(x)}{\Delta t}; \quad (4)$$

which is the well-known forward-time (Euler) scheme.

If the PDE (4) is now evaluated in $t = t^n$ you have for each $n = 0, 1, \dots, N$ the ODE:

$$\left[\frac{\partial C}{\partial t} \right] (t, x) |_{t = t^n} = -[v[l_v(t)]]_{t=t^n} \left[\frac{\partial C}{\partial x} \right] (t, x) \Big|_{t=t^n}, \forall x \in (0, 1] \quad (5)$$

Now, using the scheme type forward-time the expression (5) is transformed into:

$$\frac{C^{n+1}(x) - C^n(x)}{\Delta t} = -v(l_v^n) \frac{\partial C^n}{\partial x}(x), 0 \leq n \leq N, \forall x \in (0, 1] \quad (6)$$

Here l_v^n is the value of $l_v(t)$ in which $t = t^n$ is determined using Ruge -Kutta 4 applied to the initial problem (1)

Where, in general, $C^n(1)$ is the unknown value $C(t) = 1$ at the border $x = 1$ for time $t = t^n$. For this scheme, the known constant is the initial iteration l_v^0 . In the context of the finite differences method, the expression (6) produces an unstable numerical scheme by approximation of the spatial derivative term using a centered scheme, i.e.

$$\frac{\partial C^n}{\partial x}(x) = \frac{C_{m+1}^n - C_m^n}{\Delta x} \quad (7)$$

The instability arises because the partial derivative relative to the spatial coordinate is evaluated at a time level n earlier than the time level n where the term temporal derivative is evaluated. Therefore, a stable schema can be obtained if the two derived terms $\frac{\partial C}{\partial t}$ and $\frac{\partial C}{\partial x}$ are evaluated at the same time level n (at least a second order in Δt). In this order of ideas, Donea [1] states that the easiest way to make the evaluation of both terms of the expression (6) at the same time level n is by expressing the approximation in difference for the term of temporal derivative at the time level n . One way to achieve this is through a forward-looking Taylor serial expansion over time, including second- and third-order derivatives. That is, from the expansion

$$C(t^n + \Delta t, x) = C(t^n, x) + \Delta t \left[\frac{\partial C}{\partial x} \right] (t, x) \Big|_{t=t^n} + \frac{\Delta t^2}{2} \left[\frac{\partial^2 C}{\partial x^2} \right] (t, x) \Big|_{t=t^n} + \frac{\Delta t^3}{6} \left[\frac{\partial^3 C}{\partial x^3} \right] (t, x) \Big|_{t=t^n} + O(\Delta t^3) \quad (8)$$

The term is cleared $\left[\frac{\partial C}{\partial x} \right] (t, x) \Big|_{t=t^n}$ and (considering again the notation that was introduced for the forward-time scheme) depreciating the term $O(\Delta t^3)$ and using discretization over time (5), for the transport (4) equation can be replaced by the following:

$$\frac{C^{n+1}(x) - C^n(x)}{\Delta t} - \frac{\Delta t^2}{6} \left[\frac{\partial^3 C}{\partial t^3} \right]^n (x) = -v(l_v^n) \frac{\partial C^n}{\partial x} (x) + \frac{\Delta t}{2} \left[\frac{\partial^2 C^n}{\partial t^2} \right] (x), \forall x (0, 1] \quad (9)$$

For each $n = 0, 1, \dots, N$. The second and third derived terms that appear in this expression can be determined first by successive differentiation of the equation (4) and then by evaluating over time $t = t^n$. The calculation for the second derivative is illustrated below. On the one hand

$$\frac{\partial^2 C}{\partial t^2} = v^2 \frac{\partial^2 C}{\partial t^2} - \frac{dv}{dt} \frac{\partial C}{\partial x} \quad (10)$$

$$\frac{\partial^3 C}{\partial t^3} = v^2 \frac{\partial^2}{\partial t^2} \cdot \left(\frac{\partial C}{\partial t} \right) + 3v \frac{dv}{dt} \left(\frac{\partial^2 C}{\partial x^2} \right) - \frac{\partial C}{\partial x} \cdot \left(\frac{d^2 v}{dt^2} \right) \quad (11)$$

Now, combining (10) and (11), evaluated in $t = t^n$, with the equation (9) you have

$$\begin{aligned} & \frac{C^{n+1}(x) - C^n(x)}{\Delta t} - \frac{\Delta t^2}{6} \left[v(l_v^n) \frac{\partial^2}{\partial x^2} \left(\frac{\partial C^n}{\partial t} \right) (x) + 3v(l_v^n) \frac{dv(l_v^n)}{dt} \cdot \frac{\partial^2 C^n}{\partial x^2} (x) - \frac{d^2 v(l_v^n)}{dt^2} \cdot \frac{\partial C^n}{\partial x} (x) \right]^1 \\ & = -v(l_v^n) \frac{\partial C^n}{\partial x} (x) + \frac{\Delta t}{2} \left[v(l_v^n) \frac{\partial^2 C^n}{\partial t^2} (x) - \frac{dv(l_v^n)}{dt} \cdot \frac{\partial C^n}{\partial x} (x) \right] \quad (12) \end{aligned}$$

For everything $x \in (0, 1]$ and each $n = 0, 1, \dots, N$

The expression (12) is similar to that proposed by Leveque when generating stabilized numerical methods by dictating a diffuse term $\frac{\partial^2 C^n}{\partial x^2}$ to the nonlinear transport equation. However, it should be noted that the term $\frac{\partial^2 C^n}{\partial x^2}$ in (12) appears as part of the approximation in difference for the partial derivative of C with respect to time, evaluated at level n. On the other hand, following closely what Donea[1] suggested the term of the third-order partial derivative that appears in Taylor's serial expansion is expressed on purpose in a mixed space-time form. This mixed form of the derivative will

allow the use of type finite elements with a simple modification of the usual and consistent mass matrix quite similarly as it is done in the context of weighted residues of petrov-Galerkin. C^0 [5]

By developing the specified products and grouping the terms we have that the problem raised in (11) is semi discretized over time and for each n the next problem arises,

Given $[0,1] \ni x \rightarrow C^0(x) = C_{ini}(x)$, find, $C^n(x)_{0 \leq n \leq N}, \forall x \in [0,1]$ such that:

$$\frac{\partial^2 C^{n+1}(x)}{\partial x^2} - \alpha_1 C^{n+1}(x) = \alpha_2 \frac{\partial^2 C^n(x)}{\partial x^2} + \alpha_3 \frac{\partial C^n(x)}{\partial x} - \alpha_1 C^n(x) \quad (13)$$

$$\alpha_1 = \frac{6}{\Delta t^2 v^2} ; \alpha_2 = -2 - \frac{3\Delta t}{v} \frac{dv}{dt} ; \alpha_3 = -\frac{\Delta t}{v^2} \frac{d^2 v}{dt^2} - \frac{3}{v^2} \frac{dv}{dt} - \frac{6}{\Delta t v}$$

$$\forall x \in (0, 1] C^n(0) = C_a^n = C_a(t^n) \quad (13)$$

To be able to solve the differential equation of second order posed in (15) we need 2 conditions, but the problem only provides us with one condition so it was necessary to impose a second condition to solve the problem, which we inducted from the mathematical model for the problem of transport proper to the chemo-fluidoscillator:

$$\begin{cases} \frac{dl_v}{dt}(t) = \gamma[C(t, 1)]\{l_{eq}[C(t, 1) - l_v(t)] \Rightarrow l_v^0, C^0(x) = C_{ini}(x) \forall x \in (0, 1] \\ l_v(0) = l_v^0 \end{cases} \Rightarrow \begin{cases} l_v^{n+1} = F(l_v^n, C^n(1); \Delta t), n = 0, 1, 2, \dots, N \end{cases} \quad (14)$$

Deduction of the condition in $x = 1$

From the PDE:

$$v[l_v(t)] \frac{\partial C}{\partial x}(t, x) = -\frac{\partial C}{\partial t}(t, x) \quad (15)$$

semi-discretization of $\frac{\partial C}{\partial t} \Rightarrow \frac{C^{n+1}(x) - C^n(x)}{\Delta t}$

$$\Rightarrow v[l_v(t^{n+1})] \frac{\partial C}{\partial x}(t^{n+1}, x) = -\left[\frac{C^{n+1}(x) - C^n(x)}{\Delta t} \right]$$

$$\begin{aligned} \Rightarrow v[l_v^{n+1}] \frac{\partial C^{n+1}}{\partial x}(x) &= -\frac{C^{n+1}(x)}{\Delta t} + \frac{C^n(x)}{\Delta t} \\ \Rightarrow v[l_v^{n+1}] \frac{\partial C^{n+1}}{\partial x}(x) + \frac{C^{n+1}(x)}{\Delta t} &= \frac{C^n(x)}{\Delta t} \end{aligned} \quad (16)$$

That by evaluating her $inx = 1$, we have a Condition of Robin.

2.2 Taylor Method-Galerkin

Considering the internal product L_2 on the range: $(0,1)$

$$\langle u, v \rangle_{L_2} := \int_0^1 u(x) \cdot v(x) dx \quad (17)$$

$$\left\langle \frac{\partial^2 c(x)^{n+1}}{\partial x^2} - \alpha_1 c(x)^{n+1} - \alpha_2 \frac{\partial^2 c(x)^n}{\partial x^2} + \alpha_3 \frac{\partial c(x)^n}{\partial x} - \alpha_1 c(x)^n, v(x) \right\rangle = 0 \quad (18)$$

Applying the definition of the internal product in the spaces L_2 , with border conditions of Dirilecht and Robin, applying the integration formula in parts and replacing the functions in a way in (18) that we have for the problem:

$$\begin{aligned} &\sum_{j=1}^M c_j^{n+1} \frac{d\varphi_j(1)}{dx} \varphi_i(1) - \sum_{j=1}^M c_j^{n+1} \int_0^1 \frac{d\varphi_j(x)}{dx} \frac{d\varphi_i(x)}{dx} dx + \alpha_1 \int_0^1 \left(\sum_{j=1}^M c_j^{n+1} \varphi_j(x) \right) \varphi_i(x) dx \\ &= -\alpha_2 \sum_{j=1}^M c_j^n \frac{d\varphi_j(1)}{dx} \varphi_i(1) + \alpha_2 \sum_{j=1}^M c_j^n \int_0^1 \frac{d\varphi_j(x)}{dx} \frac{d\varphi_i(x)}{dx} dx \\ &+ \alpha_3 \sum_{j=1}^M c_j^n \frac{d\varphi_j(x)}{dx} \varphi_i(x) dx - \alpha_1 \sum_{j=1}^M c_j^n \int_0^1 \varphi_i(x) \varphi_j(x) dx \quad \forall \varphi_i, \varphi_j \in V_h \end{aligned} \quad (19)$$

2.3 Finite Element Method

We will consider a discretization of finite elements as explained above, but adapted to the working $[0,1]$ interval. In effect the partition of this interval corresponds to the longitudinal discretization of the delay line channel $(M - 1)$ into length elements $I_j = [x_j, x_{j+1}]$ for being $h_j = h$, the partition represents a mesh of points that we will denote by $x_{j+1} - x_j, j = 1, 2, 3, \dots, M. h_i = hx_j \tau_h$

If we write (19) using the elementary formulation we would have:

$$\begin{aligned}
 & \left[\begin{array}{cc} \frac{d\varphi'_i(1)}{dx} \cdot \varphi_i(1) & \frac{d\varphi'_i(1)}{dx} \cdot \varphi_{i+1}(1) \\ \frac{d\varphi'_{i+1}(1)}{dx} \cdot \varphi_i(1) & \frac{d\varphi'_{i+1}(1)}{dx} \cdot \varphi_{i+1}(1) \end{array} \right] \begin{bmatrix} C_i^{n+1} \\ c_{i+1}^{n+1} \end{bmatrix} - \left[\begin{array}{cc} \frac{d\varphi'_i(0)}{dx} \cdot \varphi_i(1) & \frac{d\varphi'_i(0)}{dx} \cdot \varphi_{i+1}(1) \\ \frac{d\varphi'_{i+1}(0)}{dx} \cdot \varphi_i(1) & \frac{d\varphi'_{i+1}(0)}{dx} \cdot \varphi_{i+1}(1) \end{array} \right] \begin{bmatrix} C_i^{n+1} \\ c_{i+1}^{n+1} \end{bmatrix} \\
 & + \frac{1}{h_i} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} C_i^{n+1} \\ c_{i+1}^{n+1} \end{bmatrix} + \frac{\alpha_1}{6} h_i \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} C_i^{n+1} \\ c_{i+1}^{n+1} \end{bmatrix} + \frac{-\alpha_{311}}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} C_i^{n+1} \\ c_{i+1}^{n+1} \end{bmatrix} [c_M^{n+1}] \\
 & = \alpha_2 \left[\begin{array}{cc} \frac{d\varphi'_i(1)}{dx} \cdot \varphi_i(1) & \frac{d\varphi'_i(1)}{dx} \cdot \varphi_{i+1}(1) \\ \frac{d\varphi'_{i+1}(1)}{dx} \cdot \varphi_i(1) & \frac{d\varphi'_{i+1}(1)}{dx} \cdot \varphi_{i+1}(1) \end{array} \right] \begin{bmatrix} C_i^n \\ c_{i+1}^n \end{bmatrix} \\
 & - \alpha_2 \left[\begin{array}{cc} \frac{d\varphi'_i(0)}{dx} \cdot \varphi_i(0) & \frac{d\varphi'_i(0)}{dx} \cdot \varphi_{i+1}(0) \\ \frac{d\varphi'_{i+1}(0)}{dx} \cdot \varphi_i(0) & \frac{d\varphi'_{i+1}(0)}{dx} \cdot \varphi_{i+1}(0) \end{array} \right] \begin{bmatrix} C_i^n \\ c_{i+1}^n \end{bmatrix} + \frac{-\alpha_2}{h_i} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} C_i^n \\ c_{i+1}^n \end{bmatrix} \\
 & + \frac{\alpha_{322}}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} C_i^n \\ c_{i+1}^n \end{bmatrix} + \frac{\alpha_1}{6} h_i \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} C_i^n \\ c_{i+1}^n \end{bmatrix} \quad (20)
 \end{aligned}$$

3.Numerical experimentation

After raising the mathematical part for the model and obtaining the system of equations, a program was designed in Matlab for the coupled system where several tests were performed with their respective numerical adjustments based on the theoretical definitions explained in chapters 2 and 3.

Each experiment details the change in the initial concentration $C(0, x) = c_{ini}(x)$ which is a unique experimental value for the operation of the hydrogel that is not listed as data in Páez[1] and has been imposed on it according to the physical model.

Experiment 1

Values are taken in the space of $M = 20$ (nodes); $dx = \frac{1}{M-1}$; $Courant = \frac{dt}{dx}$; $dt = courant \cdot dx$; $Courant = 0.1$

A constant value was taken $C(0, x) = c_{ini}(x)$ as a condition which in this case is the experimental value with which the numerical part worked in the initial study. $c_{ini}(x) = 2.2635$

The values of those derived from the concentration found in α_3 are replaced by forward differences (Euler) for $t \geq 0$

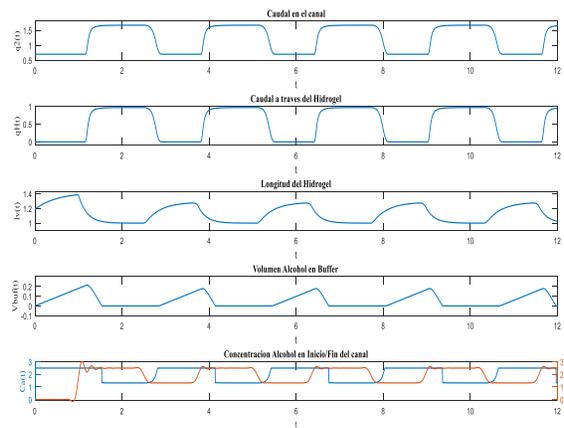


Figure 3. Response of the chemo-fluidic oscillator modeled by the system.

Periodic behavior can be observed in the Hidrogel which is what allows the device to function as an oscillator with negative feedback resulting from the increase and decrease of the alcohol mixture in the hydrogel chamber, but at the beginning of the flow of mixture of alcohol and water there is instability in the wave fronts that are then regularized as the process of opening and closing the valve progresses that because the hydrogel suffers deformation greater than the length of the camera.

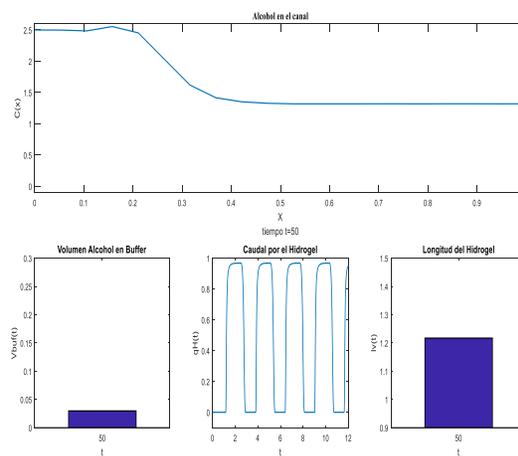


Figure 4. Response of the chemo-fluidic oscillator modeled by state variables.

Experiment 2

In this trial, a quadratic profile was taken as an initial condition since there is a mixture of water and alcohol in the canal resulting from deionized water flows and alcohol, but not reaching the minimum concentration level so that the hydrogel reacts and begins to compress due to the increase in alcohol,

periodic behavior occurs, but with less disturbance at the beginning of the process allowing a more stable and smooth concentration flow on the wave fronts.

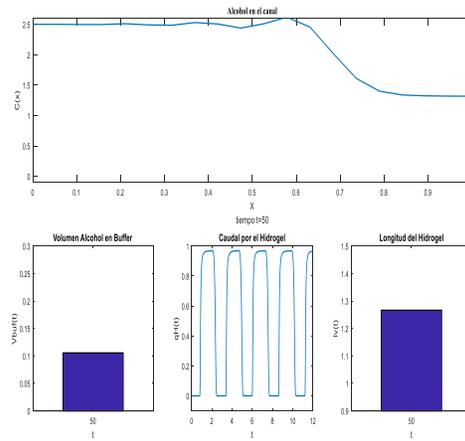


Figure 5. Response of the chemo-fluidic oscillator modeled by state variables.

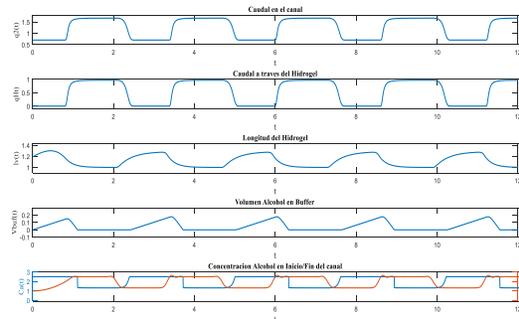


Figure 6. Response of the chemo-fluidic oscillator modeled by the system.

4. Conclusions and recommendations

The first observation that can be made is that the method applied to the system composed of (15), (16) and (17) equations reproduces the dynamics of the original numerical model of Páez[1], with small differences in amplitude and period, but that it is able to produce stable periodic signals for a parameter configuration without needing any external forcing, which means that the oscillating behavior is self-excited.

The second observation is that from a numerical approximation of the linear transport equation (constant velocity) based on the Euler-Taylor-Galerkin method for discretization over time and the Finite Elements Method for discretization in the space posed by Donea, by applying the same method with some variations in the initial conditions and border equation in the equation of the transport of the nonlinear system that is also coupled to a nonlinear ordinary differential equation that governs the

behavior of the hydrogel and another equation that controls the volume of the buffer resulting in a complex system of solving, satisfactory results were obtained in relation to its oscillation and its periodic and dimensioned movement. It is very important to note that this numerical model makes it possible to observe that if we change the initial value C_{ini} there will be a variation at the beginning of the hydrogel's operation that would be in the stationary regimen, but that after this initial regimen, the hydrogel shows an oscillating and periodic behavior typical of Páez's initial analysis.

The third observation is that this numerical analysis applied to the chemo-fluidic oscillator analytically contributes to the understanding that the valve composed of the hydrogel is extremely sensitive to the variation of the parameters, i.e. it has the ability to drastically change its volume under small variations of special thermodynamic parameters.

In this research another option could be given to mathematically model the domains of the oscillator, in the fluidic domain given by the flow network, the transport of concentration through the delay line and in the chemical domain given by the behavior of the hydrogel and the concentration of alcohol that produce a smooth dynamic system in parts.

It is recommended to use for future studies a mathematical refinement method such as the Galerkin-Discontinuous method to be able to model in more detail the behavior of the Chemo-fluidic Oscillator.

5. References

- [1] Páez Chávez, J.; Voigt, A.; Schreiter, J.; Marschner, U.; Siegmund, S.; and Richter, A. (2016). A New Self-Excited Chemo-Fluidic Oscillator Based on Stimuli-Responsive Hydrogels: Mathematical Modeling and Dynamic Behavior. *Applied Mathematical Modelling*, vol. 40(23-24), 9719-9738.
- [2] J. Donea. (1984). A Taylor-Galerkin Method for convective transport problems, *International Journal for Numerical Methods in Engineering*, vol. 20(1), 101-119.
- [3] P. D Lax and B. Wendroff. (1962). On the Stability of Difference Schemes, *Communications on Pure and Applied Mathematics*, vol. XV, 363-371.
- [4] P. D Lax and B. Wendroff. (1964). Difference schemes for hyperbolic equations with high order of accuracy, *Communications on Pure and Applied Mathematics*, vol. XVII, 381-398.
- [5] C. E. Leith. (1965). *Methods in Computational Physics*, Vol. 4. Academic Press, New York.
- [6] J. K. Dukowics and J. D. Ramshow. (1979). Tensor Viscosity Method For Convection in Numerical fluid dynamics. *Journal of Computational Physics*. Vol.32(1), 71-79.
- [7] D. Kuzmin. (2009). Explicit and implicit FEM -FCT algorithms with flux linearization, *Journal of Computational Physics*, vol. 228(7), 2517-2534.
- [8] F. Mesinger. (1977). Forward-backward Scheme and its use in a limited area model, *Beiträge zur Physik der Atmosphäre*, vol 50, 200-210.

- [9] A. Lenk, R. G. Ballas, R. Werthschützky, G. Pfeifer. (2010). *Electromechanical Systems in Microtechnology and Mechatronics: Electrical, Mechanical and Acoustic, their Interactions and Applications*. Springer-Verlag , Berlin.
- [10] R. K. Gary, A. Dixit, P. Yadav. (2009). *Basic Electronics*, Laxmi Publications , New Delhi.
- [11] A. Richter, J. Wenzel, K. Kristchmer. (2007). Mechanically adjustable chemostats based on stimuli-responsive polymers, *Sensors and Actuators B: Chemical*, vol.25(2), 569 -573 .
- [12] K. W. Morton and A. K. Parrott. (1980). Generalised Galerkin methods for hyperbolic equations. *Journal of Computational Physics*, vol.36(2), 249-270.
- [13] R. J. Leveque. (2007). *Finite Difference Methods for Ordinary and Partial Differential Equations*. Society for Industrial and Applied Mathematics.
- [14] I. Christies, D.F. Griffiths, A.R. Mitchell and O.C. Zienkiewicz. (1976). Finite element methods for second order differential equations with significant first derivatives. *International journal for numerical methods in engineering*, vol. 10, 1389-1396.