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A finite difference method formulation based on the time integral domain for the solution of Transient diffusion-advection problem

Uma formulação para o método das diferenças finitas baseado em integração no domínio do tempo para solução da equação da difusão-advecção transiente

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Marcelo Franco de Oliveira
ORCID: https://orcid.org/0000-0001-7105-5189
Federal University of Paraná, Brazil
E-mail: marcelo.franco@ufpr.br
Daniele Cristina Thoaldo
ORCID: https://orcid.org/0000-0002-3718-0477
UNIFAEL – University Center, Brazil
E-mail: danielethoaldo@hotmail.com
Rodrigo Dias
ORCID: https://orcid.org/0000-0002-5971-3414
Mechanical Engineering, Tuiuti University of Paraná
PPGECC/UFPR, Federal University of Paraná, Brazil
E-mail: rodrigo.dias@utp.br, rodrigodias@coc.ufrj.br

Resumo
Este artigo apresenta o desenvolvimento de uma formulação do Método de Diferença Finita, na solução da equação da difusão-advecção transiente. Nesta abordagem, uma função de ponderação no tempo é utilizada na equação diferencial fundamental. Assumindo uma variação linear em um intervalo de tempo, uma integração é realizada. Essa integração reduz a ordem da derivada temporal na equação básica e as condições iniciais podem ser impostas diretamente. Três problemas de transporte de poluentes são apresentados para verificar a estabilidade e a precisão da formulação proposta. Os resultados dessa formulação são comparados com os resultados dos Métodos de Elemento de Contorno. As comparações dos resultados numéricos mostram uma boa concordância entre os resultados fornecidos para com a formulação proposta e os resultados do método de elemento de contorno assumidos aqui como resultados de referência. Ao analisar os resultados pode-se concluir que a formulação apresentada neste artigo é capaz de produzir resultados precisos para o problema.
Palavras-chave: aproximação numérica. método das diferenças finitas. difusão-advecção. dispersão de poluentes.

Abstract
This paper is concerned with the development of a formulation of the Finite Difference Method, in the solution of the transient diffusion-advection equation. In this approach, a weighting function with respect to time is used in the fundamental differential equation. By assuming a linear variation in some time interval, a time integration is performed. This integration reduces the order of time derivative in the basic equation and the initial conditions can be taken into account directly in consequence. Three pollutant transport problems are presented in order to verify the stability and accuracy of the proposed approach. The results for this approach are compared with the Boundary Element Methods results. The comparisons of numerical results show a good agreement between

the furnished results for the proposed approach and the boundary element method results assumed here as reference results. By analyzing the results one can conclude that the formulation presented in this paper is capable of producing accurate results for the problem.
Keywords: numerical approach. finite difference method, diffusion-advection. pollutant dispersion.

Table 1: List of the symbol used on the paper.

k – Index that represent the discrete time.	α - Constant in the formulation.
i – Index that represent the discrete domain.	β - Constant in the formulation.
T – Time Integral.	γ - Constant in the formulation.
t_0 - Initial time.	λ - Constant in the formulation.
t_f - Final time.	P_e - Péclet number.
K - Represents the first order decay.	U_0 - Boundary condition for potential at $x=0$.
$u(x,t)$ - Concentration substance of interest.	q_0 - Boundary condition for flux.
D - Diffusion coefficient.	U_L -Boundary condition for potential ate $x=L$
V - Depth-averaged horizontal velocity.	$U_0(t)$ - Variable boundary condition.
$w(t)$ - Weighting function in time.	T_0 - Initial conditions.
t_n, t_{n+1} - Discretization time.	L - Length of the channel.
$\phi(t)$ - Interpolation function.	ψ - Constant in the formulation.

1. Introduction

Pollutant transportation and dispersion is a very important environmental problem in present days, and it can be described by the diffusion-advection equation (Scott & Gerhard, 2002). The equation diffusion-advection in environment problems is a good justify, to find ways of the numerical solutions aiming minimizing computational time process involved in solutions of the practical problem. The control of the water source pollution is an important ally for the implementation of prevention measures concerning the environmental health (Cunha, et al., 2013). As a consequence, a great number of formulations has appeared in the last few years enriching the literature concerning in this matter. This work presents an approach for the Finite Difference Method - FDM formulation for the solution of the diffusion-advection equation. This formulation employs a constant weighing function in time, and the differential equation is first numerically integrated from the initial time t_0, to a specified final time t_f. By applying this approach directly in the governing equation, it gave a quite original formulation. Over each time interval in a feature that can be identified as the subdomain collocation (Finlayson Bruce, 1972), so the formulation is called here FDM-T where T referrers the time integral. As a matter of fact, the reliable and accurate results presented by Carrer & Mansur (2010) and Carrer, et al. (2012) using Boundary Element Methods (BEM) with a similar approach to solve transient wave and heat equation respectively, encourage the author to develop this work. In addition, Oliveira (2020) makes use of the same approach for the finite difference method in order to solve pure diffusion problem. The accurate reached results encouraged the author in the seek for new applications. It is important to mention that the time integration in the basic equation, reduces the order of time derivative and the initial conditions can be imposed directly. With the aim to verify the result's potentialities for the presented approach, three examples are presented and discussed in this article. To ensure the confiability of results for this approach, the Boundary Element Method is used to compare and validated the results. The BEM has been successfully applied in the analysis of diffusion-advection equation in the last few years e. g. (Carrer, et al., 2017, Pettres, et al., 2015 and Cunha, et al., 2013), as pure diffusion problems see Carrer, et al. (2012), Ochiai, et al. (2006) and Pettres, et al. (2015). Numerical methods and theory of solutions of the problems for differential equations using FDM have been studied extensively by many researchers (Liu, Cheng, & Li Xiaoli, 2018), (Čiegis & Subоč, 2018) and so on. From the academic point of view, the development of alternatives approaches and formulations for the same method enriches and broadens the discussion about the method. Also, this discussion enlarges its range of applications. Concerning the numerical solution of the problem, the FDM has been successfully used. The following works can be mentioned: the FDM formulation for two-dimensional equation is presented by (Cunha & Rosman, 2018), a study concerning the stability is presented by (Dai & Johnson, 2010), a high accuracy adaptive difference strategy on 1D reaction-diffusion equation with convection in (Zhu & Hongxing, 2019). The coupling of finite element method (FEM) with FDM, and boundary element method with FDM is also successfully used, Wang & Zhen-Hui (2005) and Cunha et al. (2018) used FEM in spatial, Carrer et al. (2017) used BEM in spatial, and those papers used FDM in temporal discretization. Although the numerical aspects of this equation are a very attractive field, the applicability for this problem is also a very important issue in engineering. The diffusion-advection equation that describes heat and mass transfer has been widely applied in the thermal field such as skin burn (Dai, Yu and Nassar, 2004), two-dimensional (2D) incompressible fluid flow problems with heat transfer is presented by Zamolo & Nobile (2019). Concerning the diffusion-advection equations, it has been successfully studied in many numerical applications as the fractional space via radial basis (Zafarghandi & Mohammadi, 2019), new approximation on non-uniform meshes (Soori & Aminataei, 2019) among others.

2. Material and Methods

2.1. Mathematical Model

The basic one-dimensional governing diffusion-advection equation, over a domain Ω and limited by a boundary Γ, is given by:

$$D \cdot \frac{\partial^2 u(x,t)}{\partial x^2} - V \cdot \frac{\partial u(x,t)}{\partial x} - K \cdot u(x,t) = \frac{\partial u(x,t)}{\partial t} \tag{1}$$

Where D and V are assumed constant in this work, both in space and in time. In this work is considered $K = 0$. A deeper discussion about equation (1) and its coefficients, can be found in Cunha, et al. (2006) and Cunha, et al. (2018).

2.2. FDM Formulation (Rapp, 2017)

By following the basic procedures for the FDM, see the textbooks by Greenberg, (1988) and Gordon, (1985) for the explicit progressive numerical scheme and applying in equation (1), the basic equation is rewritten below:

$$\frac{D}{\Delta x^2}\left(u_{i-1}^{k} - 2u_i^k + u_{i+1}^k\right) - \frac{V}{\Delta x}\left(u_{i+1}^k - u_i^k\right) = \frac{1}{\Delta t}\left(u_i^{k+1} - u_i^k\right) \tag{2}$$

where k represents the time and i represents the point in the domain. In equation (2), the solution is obtained in an explicit form. Due to the combination of two effects, diffusive and advective the explicit method is sensitive for the choice of Δt. The relationship between these two effects is named as Péclet Number (Cunha C. , Carrer, Oliveira, & Viviane, 2016).

$$P_e = \frac{V \cdot \Delta x}{D} \tag{3}$$

According to Rapp (2017) the value of Péclet number, the equation has diffusion-dominated processes for low, or convection-dominated processes, for high. Generally, standard or explicit numerical methods can easily solve the diffusion-dominated but not the convection-dominated, in which case oscillations and smoothing of the propagating front may develop (Qiu, Wrobel, & Power, 1998).

2.3. FDM-T formulation

For this approach, let's say in the time interval $t_n \le t \le t_{n+1}$ a weighting function $w(t)$ satisfy the equation:

$$w(t) = \begin{cases} 1, & t_n \le t \le t_{n+1} \\ 0, & t \notin [t_n, t_{n+1}] \end{cases} \tag{4}$$

Using the subdomains collocation principle, a time integral is carrying out in the time interval given by (4), therefore the equation (2) is rewritten as:

$$\frac{D}{\Delta x^2}\int_{t_0}^{t_f} w(t)\cdot(u_{i-1}^k - 2u_i^k + u_{i+1}^k)dt - \frac{V}{\Delta x}\int_{t_0}^{t_f} w(t)\cdot(u_{i+1}^k - u_i^k)dt = \frac{1}{\Delta t}\int_{t_0}^{t_f} w(t)\cdot\frac{\partial u(x,t)}{\partial t}dt \tag{5}$$

Time integration is restricted to the time interval, in this interval the function $u(x,t)$ has a linear variation as follows:

$$u(x,t) = \phi(t_n)u(x,t_n) + \phi(t_{n+1})u(x,t_{n+1}) \tag{6}$$

In this work a constant time interval was used, so the interpolation function is equal 1. If the time interval is not constant, the interpolation fiction is

$$\phi(t_n) = \frac{t_{n+1} - t}{\Delta t} \text{ and } \phi(t_{n+1}) = \frac{t - t_n}{\Delta t} \tag{7}$$

After substituting (6) in (5) and performing integration, gives

$$u_{i-1}^k - u_i^k + u_{i+1}^k + u_{i-1}^{k+1} - u_i^{k+1} + u_{i+1}^{k+1} - \alpha\left[u_{i+1}^k - u_i^k + u_{i+1}^{k+1} - u_i^{k+1}\right] = \beta\left[u_i^{k+1} - u_i^k\right] \tag{8}$$

with

$$\alpha = -\frac{V \cdot \Delta x}{D} = -P_e \tag{9}$$

and

$$\beta = \frac{2\Delta x^2}{D \cdot \Delta t} \tag{10}$$

Rearranging the equation (8), one has:

$$u_{i-1}^{k+1} + \gamma \cdot u_i^{k+1} + \lambda \cdot u_{i+1}^{k+1} = -u_{i-1}^{k} + (1-\alpha-\beta)\cdot u_i^k - \lambda \cdot u_{i+1}^k \tag{11}$$

where $\gamma = \alpha - \beta - 1$ and $\lambda = 1 - \alpha$.

From the equation (11) a tridiagonal system of equations is generated

$$\begin{bmatrix} \gamma & \lambda & 0 & 0 & 0 & 0 & 0 \\ 1 & \gamma & \lambda & 0 & 0 & 0 & 0 \\ 0 & 1 & \gamma & \lambda & 0 & 0 & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 1 & \gamma & \lambda \\ 0 & 0 & 0 & 0 & 0 & 1 & \gamma+\lambda \end{bmatrix} \begin{bmatrix} u_1^{k+1} \\ u_2^{k+1} \\ u_3^{k+1} \\ . \\ . \\ u_{n-1}^{k+1} \\ u_n^{k+1} \end{bmatrix} =$$

$$\begin{bmatrix} 1-\alpha-\beta & -\lambda & 0 & 0 & 0 & 0 & 0 \\ -1 & 1-\alpha-\beta & -\lambda & 0 & 0 & 0 & 0 \\ 0 & -1 & 1-\alpha-\beta & -\lambda & 0 & 0 & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & -1 & 1-\alpha-\beta & -\lambda \\ 0 & 0 & 0 & 0 & 0 & -1 & 1-\alpha-\beta \end{bmatrix} \begin{bmatrix} u_1^{k} \\ u_2^{k} \\ u_3^{k} \\ . \\ . \\ u_{n-1}^{k} \\ u_n^{k} \end{bmatrix} - \begin{bmatrix} u_0^{k} \\ 0 \\ 0 \\ . \\ . \\ 0 \\ q_0 \end{bmatrix} \tag{12}$$

It is important to point out, with the approaches developed here the solution is obtained in an explicit form. A reduction for the nodal error is achieved, as a consequence, it can provide a reduction in the number of interactions for the solution.

3. Results

3.1. Numerical Examples

In this section, three different examples are presented to show how this approach can be applied to solve diffusion-advection problems. All three examples consist of a one-dimensional channel with a size of *L*, in example 1 and 2 a continuous source in boundary *x=0*, in the example 3, a time variable source is applied. The domain discretization consists in $\Delta x = 0.75m$, and *L=12m*. The following parameters were adopted: $V = 0.05m/s$, $V = 0.0375m^2/s$ and $\Delta t = 0.5s$.

To assess the potentialities of the FDM-T formulations, the results are compared with the BEM formulation, which is assumed as the exact solution to verify consistency, convergence e stability. The BEM formulation used in order to validate the FDM-T approach has been used in several studies with numerical and analytical validations. Recent works can be motioned such as Pettres, Lacerda, & Carrer (2015) applied the BEM formulation for the pure diffusion problem, and the numerical results were validated with the analytical solution and linear regression was applied to evaluate the correlation between the solutions. Also, Carrer, Cunha, & Mansur (2017) present a study for two-dimensional diffusion-advection equation using BEM for non-isotropic material. In this work, the numerical results were validated with the analytical solution showing the effectiveness of the method. And for last but not less important Carrer et al. (2021) present a numerical study for two-dimensional diffusion-advection problems with a spatially variable velocity field. In this paper, the author presents the first example in which the analytical solution is well known, and the numerical results for BEM are very accurate, although in the second example no analytical solution is available for the problem; then the comparison for BEM results was carried out with the FEM results.

3.1. Example 1 - Channel with flux prescribed at the end

This example consists in a channel with a length equal to *L*, subject to the following boundary and initial conditions

$$u(0,t)=U_0 \tag{13}$$

$$\frac{\partial u(L,t)}{\partial x}=q_0 \tag{14}$$

$$u(x,0)=T_0 \tag{15}$$

The equation (14) represents the flux in the selected point. Adopting $U_0=1$, $q_0=0$ and $T_0=0$, three points in the domain were selected and the results in these points are depicted in the figure 1. The points are $A(L/4)$, $B(L/2)$ and $C(3L/4)$.

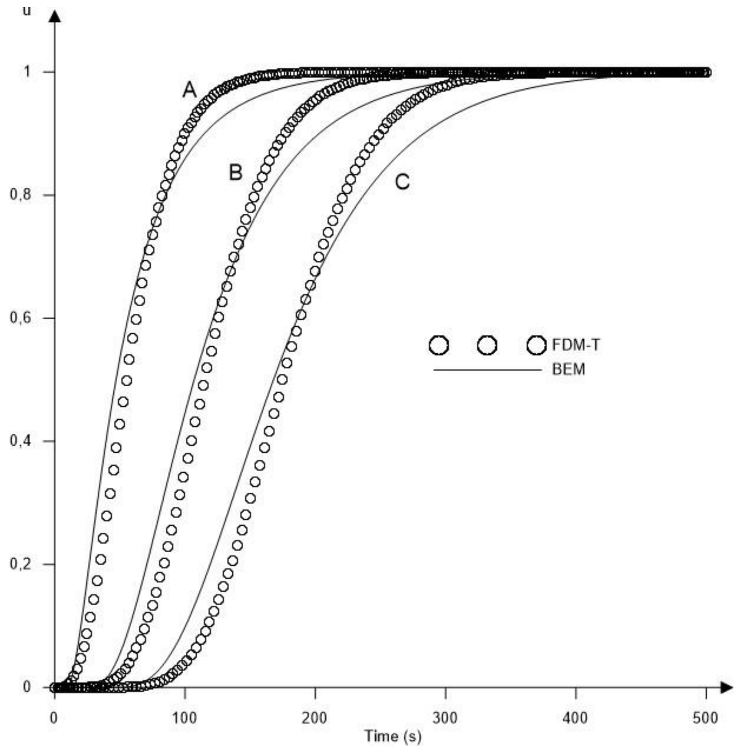

Figure 1 – Concentration in the three selected points.

A good agreement between solutions from BEM and FDM-T is observed in Figure 1 . It is possible to observe that the results are stable and convergent, thus confirming that the FDM-T formulation is adequate for such kind of analysis. As to the accuracy, the FDM-T curves are more diffused than the BEM one. In other words, the FDM-T formulation introduces some artificial diffusion. The figure 2 presents the errors for the selected points.

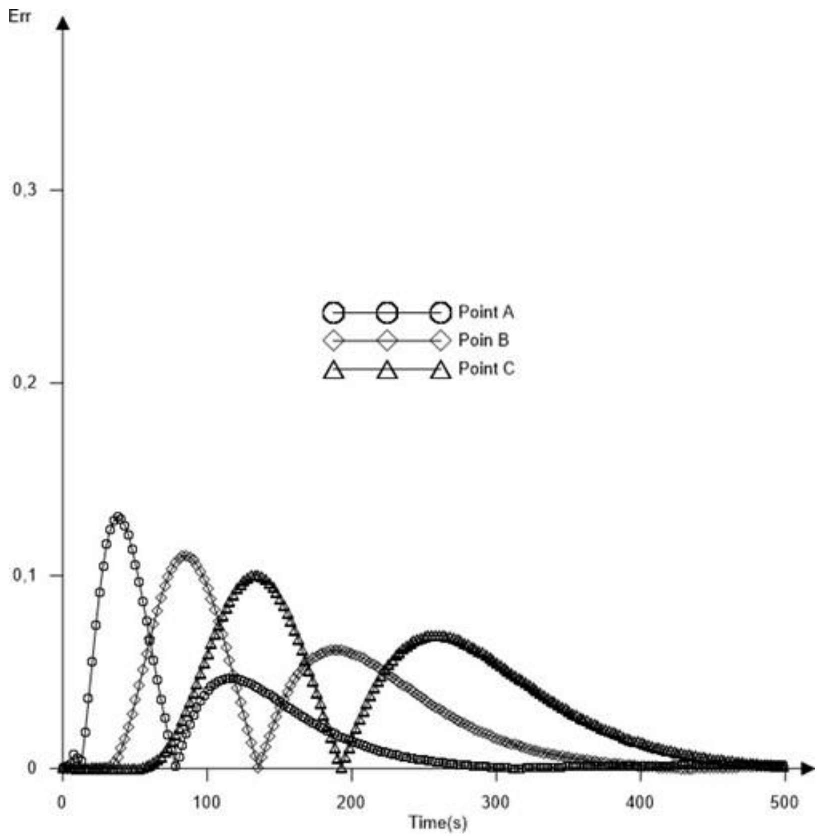

Figure 2 –Error between FDM-T and BEM results.

Far from intending to carrying out a profound error analysis discussion, the use of error enables to verify convergence and accuracy for numerical results. From figure 2 , it is observed the error decay over time, but in initial times a divergence in order of 10^{-1} is observed. Anyway, the use of more refined meshes produces more accurate results and smaller errors. The next figure shows a graphic for this example using the diffusion coefficient equal to 2. With $D = 2m^2/s$ and $V = 0.1m/s$ the Péclet number is $Pe = 0.0375$, in this way the problem is diffusion-dominated. In this graphic, the points A and B are depicted. It is possible to observe in figure 3 , the BEM and FDM-T results are in good agreement. Comparing figure 3 with figure 1 is important to mention that the difference between both formulations is lower when diffusion is dominant in the problem.

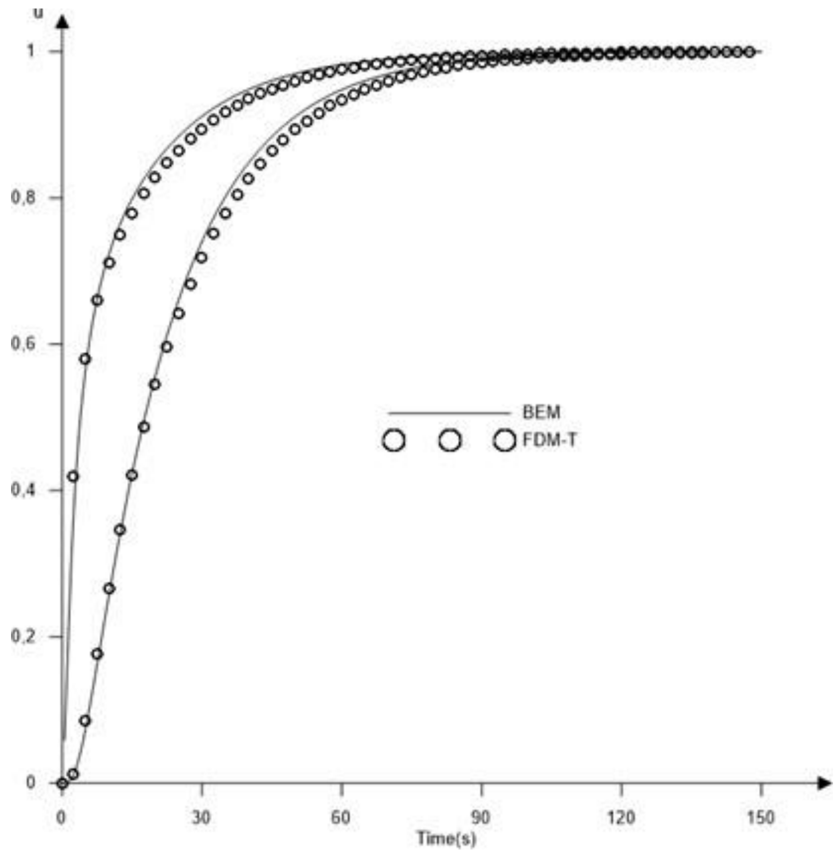

Figure 3 – Concentration with D = 2m^2/s and V=0.1 m/s.

3.2. Example 2 - Channel With Prescribed Concentration in Both Ends

In this example, a continuous concentration is prescribed in both sides of the channel. The following equations represent the boundary and initial conditions.

$$u(0,t) = U_0 \tag{16}$$

$$u(L,t) = U_L \tag{17}$$

$$u(x,0) = T_0 \tag{18}$$

Applying (17) in (11) the equations system (12) is rewrite as

$$\begin{bmatrix} \gamma & \lambda & 0 & 0 & 0 & 0 & 0 \\ 1 & \gamma & \lambda & 0 & 0 & 0 & 0 \\ 0 & 1 & \gamma & \lambda & 0 & 0 & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 1 & \gamma & \lambda \end{bmatrix} \begin{bmatrix} u_1^{k+1} \\ u_2^{k+1} \\ u_3^{k+1} \\ . \\ . \\ u_{n-1}^{k+1} \end{bmatrix} =$$

$$\begin{bmatrix} 1-\alpha-\beta & -\lambda & 0 & 0 & 0 & 0 & 0 \\ -1 & 1-\alpha-\beta & -\lambda & 0 & 0 & 0 & 0 \\ 0 & -1 & 1-\alpha-\beta & -\lambda & 0 & 0 & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & -1 & 1-\alpha-\beta & -\lambda \end{bmatrix} \begin{bmatrix} u_1^{k} \\ u_2^{k} \\ u_3^{k} \\ . \\ . \\ u_{n-1}^{k} \end{bmatrix} - \begin{bmatrix} u_0^{k} \\ 0 \\ 0 \\ . \\ . \\ \lambda u_n^{k} \end{bmatrix} \quad (19)$$

Adopting $U_0 = 1$, $U_L = 0$ and $T_0 = 0$, the same points are depicted in the figure 4. The points are $A(L/4)$, $B(L/2)$ and $C(3L/4)$.

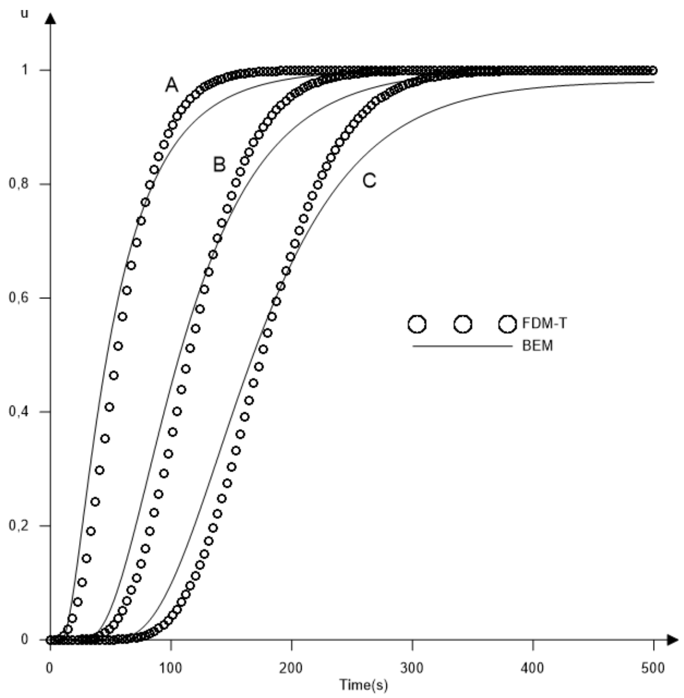

Figure 4 – Concentration in the three selected points.

Again, as can be observed in figure 4 a good agreement is achieved with FDM-T approaches. The results show good convergence and stability. Regarding the accuracy, the major difference is observed between 200 and 300 seconds, which can be considered acceptable taking into account that the FDM-T results do present neither overshoot nor oscillatory behavior. A remark concerning the selection of the time-step is necessary for this discussion. As the time-step has an important role in the numerical solution of transient problems and the use of smaller values of Δt is not necessarily followed by more accurate numerical solutions (Carrer, Cunha, & Mansur, 2017). Also is important to mention the time step used in the present paper is less than 1 second. In the diffusion-convection study presented by Cunha, et al., (2016) the autos use 4 seconds in the boundary element analysis and 1 second in the finite element analysis. But in a similar study given by Carrer, et al., (2017) to achieve good results the authors use a time-step equal to 0.1 and 0.025 seconds. Therefore, the time step used here is in conforming, or even better with the literature concerning about this matter.

3.3. Example 3 - Channel With a Time Variable Boundary Condition

In this example is used the same parameter as example 1, but the boundary condition at $x = 0$ is given by the following equation:

$$u(0,t) = U_0(t) \tag{20}$$

with $U_0(t) = \psi\left(1 - \cos(\omega \cdot t)\right)$ where ψ is a constant, assumed here equal 0.5. This is a very interesting example since the steady state condition is never reached due to the time-dependent boundary condition. This problem is very effective to test stability and convergence for the numerical methods. A discussion concerning this example for the pure diffusion equation can be found in 7 and 4. In fact, the accurate results presented by these authors were a motivation for including this example as a test to the proposed approach.

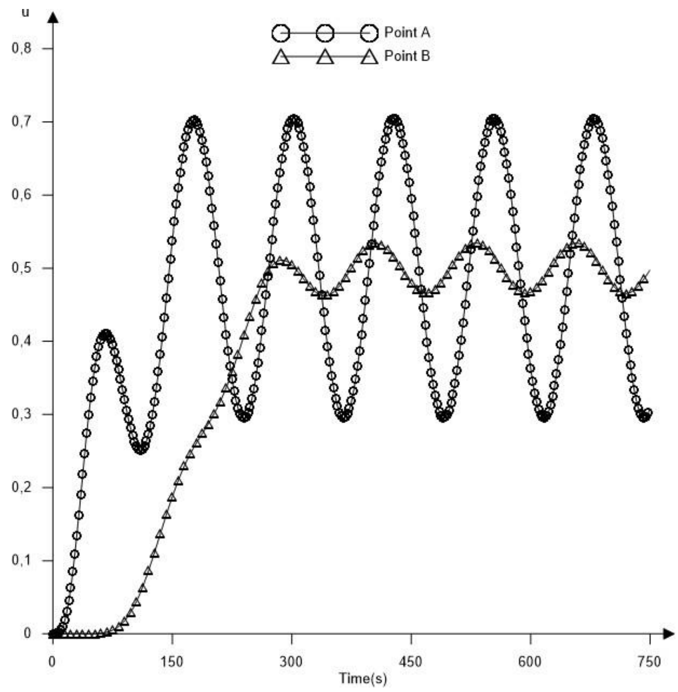

Figure 5 –Concentration with variable boundary condition.

For this example, only the FDM-T is depicted in figure 5. The main purpose of this problem is to test the stability and convergence for this approach. The results for two points are presented, $A(L/4)$ and $B(3L/4)$. It is possible to see in figure 5 that the results for this example are consistent with regard to stability and convergence.

4. Conclusions

With the purpose to enlarge and enrich the range of applications and discussion about the numerical solution for diffusion-advection problems, an alternative FDM approach were presented in this work, namely the FDM-T. This approach demonstrated to be usefulness in diffusion-advection problems. The alternative approaches employing a time integral brings a reduction in the order of time derivative of equation, and the initial conditions could be impose directly. By using subdomain collocation method, it gave a quite original formulation which is called here as FDM-T. The three numerical examples presented here validate the results and demonstrates the stability, convergence, and accuracy are reliable. This approach can be extended to nonlocal boundary value problems with more complicated conditions without substantial efforts. Although the approach is only illustrated here for one-dimensional problems, its extension to similar two-dimensional problems is straightforward. For this reason, the author’s conclusion is that the proposed approach looks very promising, and based on the results obtained in this approach it’s appropriate and can be used quantitatively to study the phenomenon of diffusion-advection transportation.

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