A TIME-DOMAIN BOUNDARY ELEMENT METHOD FORMULATION FOR ADVECTION-DIFFUSION PROBLEMS

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Abstract. *This work is concerned with the development of a time-domain Boundary Element Method formulation for the solution of the advection-diffusion problem in twodimensions. It is important to point out that the problem to be solved has become very important nowadays: if one bears in mind that the advection-diffusion equation describes problems such as pollutants dispersion, then the development of a formulation capable of dealing with this social and environmental problem is welcome. In order to verify the accuracy of the proposed formulations, one example is presented and discussed.*

Keywords: *Advection-diffusion equation, TD-BEM, Time-domain BEM, Pollutants dispersion*

1 INTRODUCTION

The advection-diffusion equation describes an important environmental problem, that is, the problem of the pollution dispersion; consequently, it can be employed as a support in the choice of strategic decisions in what concerns sewage effluent in rivers and in coastal areas. Due to the growing importance of the problem, the development of numerical and analytical models for the solution of the problem is plainly justified.

With respect to the numerical solution of the problem, the Finite Difference Method (FDM) and the Finite Element Method (FEM) have been successfully used during the last years. The following references can be cited: Zhao et al. (1994); Ataie-Ashtiani and Hosseini (2005); Prieto et al. (2011); Dhawan et al. (2012).

With the purpose of contributing with the discussion concerning the solution of the advection-diffusion equation, a Boundary Element Method (BEM) formulation is presented in this article. Different BEM formulations arise according to the fundamental solution employed in obtaining the basic integral equation of the method, see Polyanin (2002) for a very complete set of fundamental solutions. This characteristic of the method turns the analysis of time-dependent problems very attractive.

In a broad sense, the BEM formulations, for the solution of time-dependent problems, can be classified according to: D-BEM with D meaning domain, DR-BEM with DR meaning dual reciprocity and TD-BEM with TD meaning time-domain. The D-BEM and the DR-BEM formulations have a common origin, that is, both employ the fundamental solution corresponding to the steady-state problem. The basic integral equation of the method, for this reason, presents a domain integral, whose kernel is constituted by the steady-state fundamental solution multiplied by the first order time derivative of the substance. The transformation of the domain integral into boundary integrals, by means of suitable interpolation functions, generates the so-called DR-BEM formulations, e.g. Singh and Tanaka (2003). If the domain integral is kept in the integral equation, then the D-BEM arises, e.g. Taigbenu and Liggett (1986), Carrer et al. (2012), Pettres et al. (2015). Note that the discretization of the entire domain is required. The choice of a time-marching scheme or, in other words, the choice of the approximation for the first order time derivative of the substance, is necessary for both the DR-BEM and the D-BEM formulations.

The TD-BEM formulation employs time-dependent fundamental solutions and is the formulation presented in this work. As a consequence, the solution of problems with homogeneous initial condition requires only the boundary discretization, whereas the presence of non-homogeneous initial condition requires only the discretization of the part of the domain where it occurs, e.g. Wrobel (1981). The main criticism for the TD-BEM formulation is the high computational cost involved in the assemblage of the matrices.

An already classical example is included. It consists of a one-dimensional transport problem in a semi-infinite medium, which has an analytical solution, see Ogata and Banks (1961). The TD-BEM results are compared with the available analytical solution, enabling one to assess the potentialities of the TD-BEM formulation.

2 THE ADVECTION-DIFFUSION PROBLEM

The two-dimensional depth-integrated advection-diffusion problem, over a domain Ω limited by a boundary Γ, is governed by the equation below, Taigbenu and Liggett (1986):

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right], \tag{1}$$

where $C(X,t)$, the concentration of the substance of interest, is treated as a function of space and time, in which X represents the point of coordinates (x,y), U and V are the depth-averaged components of the horizontal velocity and D is the diffusion coefficient.

2.1 Boundary and Initial Conditions

There are two kinds of horizontal boundaries: land boundaries and open boundaries. In general, land boundaries represent the margins of the water body and possible points with inflows or outflows, such as rivers. Open boundaries usually represent water domain limits, such as the entrance of a bay or estuary, and not a physical boundary. Along open boundaries, it is usual to neglect the diffusive fluxes and the transport equation is taken into account with no diffusive terms along the boundary points. The prescription of normal fluxes is associated with land boundaries.

The general land boundary condition can be written as:

$$U_n C - D\frac{dC}{dn} = F_n^*, \tag{2}$$

where the subscript n stands for normal direction and F_n^* is normal flux.

Quite often, U_n and F_n^* are zero and, therefore, the above equation is reduced to:

$$\frac{dC}{dn} = 0 \tag{3}$$

In the case of significant inflows ($U_n < 0$), such as a river or a small estuary that ends in a bay, the normal flux along the segment has to be specified, resulting in the following condition:

$$U_n C = F_n^*. \tag{4}$$

The part of domain related to Eq. (3) is denoted as Γ_Q whereas the part related to Eq. (4) is denoted as Γ_C, which means that $\Gamma = \Gamma_Q \bigcup \Gamma_C$.

The initial conditions, over the domain Ω, are:

$$C(X,0) = C_0(X). \tag{5}$$

3 TD-BEM FORMULATION

By following a procedure based on the method of the weighting residuals, see, for instance, the textbooks by Brebbia et al. (1984), Zienkiewicz and Morgan (1983), Brebbia and Connor (1977), Fynlaison (1972), the BEM formulations differ according to the fundamental solution, Polyanin (2002), employed as the weighting function. In the TD-BEM formulation, the fundamental solution is no longer the fundamental solution of the related steady-state problem, but is the solution of the time-dependent problem, that is, the fundamental solution is the solution of the equation:

$$D\nabla^2 u^*(\xi,\tau,X,t) + U\frac{\partial u^*(\xi,\tau,X,t)}{\partial x} + V\frac{\partial u^*(\xi,\tau,X,t)}{\partial y} + \frac{\partial u^*(\xi,\tau,X,t)}{\partial \tau} = -\delta(X-\xi)\delta(t-\tau). \quad (6)$$

The expression of the time-dependent fundamental solution is presented by Li and Evans (1991) without the non-conservative term. With the non-conservative term included, it reads:

$$u^*(\xi,\tau,X,t) = \frac{e^{-\frac{r^2}{4D(t-\tau)}}}{4\pi D(t-\tau)} e^{-g(\xi,\tau,X,t)}, \quad (7)$$

where

$$g(\xi,\tau,X,t) = \frac{U}{2D}(x-\xi_x) + \frac{V}{2D}(y-\xi_y) + \left(\frac{U^2+V^2}{4D}\right)(t-\tau). \quad (8)$$

The TD-BEM integral equation is written as follows:

$$c(\xi)C(\xi,t) = D\int_\Gamma \int_0^t u^*(\xi,\tau,X,t)Q(X,t)d\tau d\Gamma(X) - D\int_\Gamma \int_0^t \left[q^*(\xi,\tau,X,t) + \left(\frac{Un_x+Vn_y}{2D}\right)u^*(\xi,\tau,X,t)\right]C(X,t)d\tau d\Gamma(X) + \int_\Omega u^*(\xi,\tau,X,t)C_0(X)d\Omega(X). \quad (9)$$

The coefficient $c(\xi)$, on the left-hand-side of Eq. (9) is computed according to:

$$c(\xi) = \frac{\alpha}{2\pi}, \quad (10)$$

where α is the angle depicted in Fig. 1. For internal points ($\xi \in \Omega$), one has $c(\xi) = 1$.

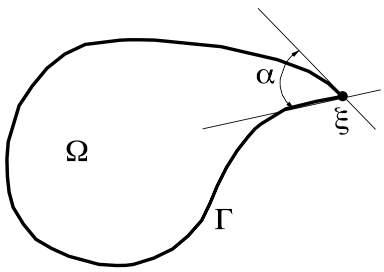

Figure 1: Internal angle α used in the computation of the coefficient $c(\xi)$.

The time integrals that appear in Eq. (9) are convolution integrals and the domain integral is restricted only to the part of the domain which presents non-null initial conditions.

The function $q^*(\xi,\tau,X,t)$, which appears in the kernel of the second integral on the right-hand-side of Eq. (9), is given by:

$$q^*(\xi,\tau,X,t) = -\frac{r}{2D(t-\tau)}\frac{e^{-\frac{r^2}{2D(t-\tau)}}}{4\pi D(t-\tau)}e^{-g(\xi,\tau,X,t)}\frac{dr}{dn(X)}. \tag{11}$$

The domain integral is restricted only to the part of the domain which presents non-homogeneous initial conditions. Naturally, if the problem presents null initial conditions, the numerical analysis is restricted to the boundary of the problem.

The application of the discretized version of the boundary integral equation to all boundary nodes produces the system of algebraic equations written below:

$$H^{nn}C^n = G^{nn}Q^n + \sum_{m=0}^{n-1}(G^{nm}Q^m - H^{nm}C^n) + F^nC_0. \tag{12}$$

Note that the convolution integral from the initial time t_0 the current time t_n generates the summation indicated in Eq. (12).

In Eq. (12), the superscript n is associated with time $t_n = n\Delta t$, $n \geq 1$, and the superscripts m, to the times t_m previous to t_n.

The contaminant and its normal derivative are assumed as constant functions of time inside each time interval. In fact, this is the simplest possible choice and, even so, capable of producing accurate results. Time integrals are evaluated numerically, as $u^*(\xi,\tau,X,t) \to 0$ when $\tau \to t$. The integral containing $u^*(\xi,\tau,X,t)$ along each element (singular or not) is also evaluated numerically. Singular integrals containing $q^*(\xi,\tau,X,t)$ are null because, as already mentioned, $\frac{dr}{dn} = 0$ for linear elements. The integration of the cells is carried out analytically in the radial direction and numerically in the angular direction when the aforementioned system of polar coordinates with pole in the source point is adopted.

For additional details concerning the computation of the convolution integrals, as well as cell integration, the reader is referred to Wrobel (1981) and Mansur (1983).

4 EXAMPLE: 1-D SEMI-INFINITE CHANNEL

The example consists of a semi-infinite one-dimensional channel aligned with the x-axis and with uniform U. The boundary and initial conditions are:

$$\begin{aligned} &C(x,0) = 0 \quad \text{for} \quad t = 0 \\ &C(0,t) = C_0 \quad \text{for} \quad t > 0 \\ &C(\infty,t) = 0 \quad \text{for} \quad t > 0. \end{aligned} \tag{13}$$

The analytical solution for this one-dimensional flow problem is written below, see Ogata and Banks (1961), but can be found, for instance, at Taigbenu and Liggett (1986), Wang et al. (2012). It reads:

$$C(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x-Ut}{2\sqrt{Dt}}\right) + \operatorname{erfc}\left(\frac{x+Ut}{2\sqrt{Dt}}\right)e^{\frac{Ux}{D}}\right], \tag{14}$$

where erfc(..) is the complementary error function.

The numerical analyses were carried out on a rectangular finite domain with length $L = 12m$ and height $H = 6m$, in such a way that: $0 \leq x \leq L$ and $0 \leq y \leq H$. As it is well known, the Peclet number, defined according to (Δx is the reference length):

$$Pe = \frac{U\Delta x}{D}, \tag{15}$$

characterizes the nature of the transport, that is: for $Pe < 1$, the diffusion is dominant; for $Pe = 1$, the diffusion and the advection are equally dominant and for $Pe > 1$, the advection is dominant.

The following parameters were adopted: $U = 0.05m/s$ and $V = 0$. The analyses were carried out, initially, with the mesh depicted in Fig. (2) (96 boundary elements).

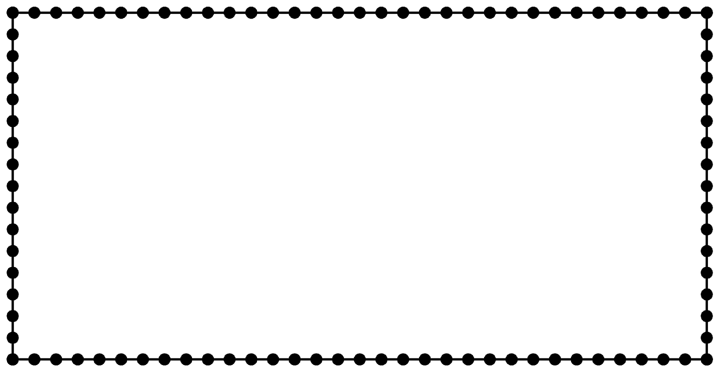

Figure 2: Boundary discetization.

To assess the potentialities of the BEM formulations, four Peclet numbers, related only to the dominant advection case, were adopted. This is justified as this case is the worst to be solved numerically. By adopting $D = 0.00375m^2/s$, one has $Pe = 5$. The other diffusion values are: $D = 0.001875m^2/s$, $0.0009375m^2/s$, $0.00046875m^2/s$, corresponding, respectively, to $Pe = 10$, 20, 40, because $\Delta x = 0.375m$. The results related to the contaminant along the x-axis, for $t = 20s$, $60s$, $100s$, $140s$, $180s$, are depicted from Fig. (3) to Fig. (6), from the lower to the higher Pe number. Bearing in mind that a channel with finite length is employed in the numerical analyses, for the selected time values the boundary condition $C(\infty, t) = 0$ is satisfied at $x = L$.

A remark concerning the selection of the time-step, Δt, becomes necessary at this point of the discussion. The time-step plays 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 in TD-BEM formulations (this statement becomes clear in the TD-BEM for elastodynamics, see Mansur (1983)); as a consequence, the researcher experience also plays an important role in the time-step selection. Following this reasoning, several analyses, not included here, were carried out until reaching the value $\Delta t = 2s$, which produced reliable results.

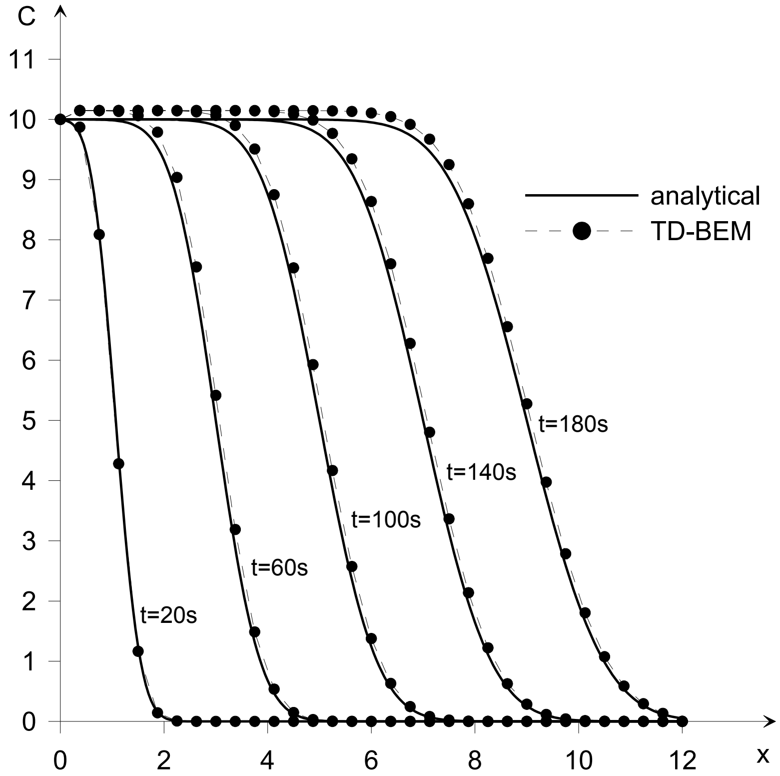

Figure 3: Results for $Pe = 5$.

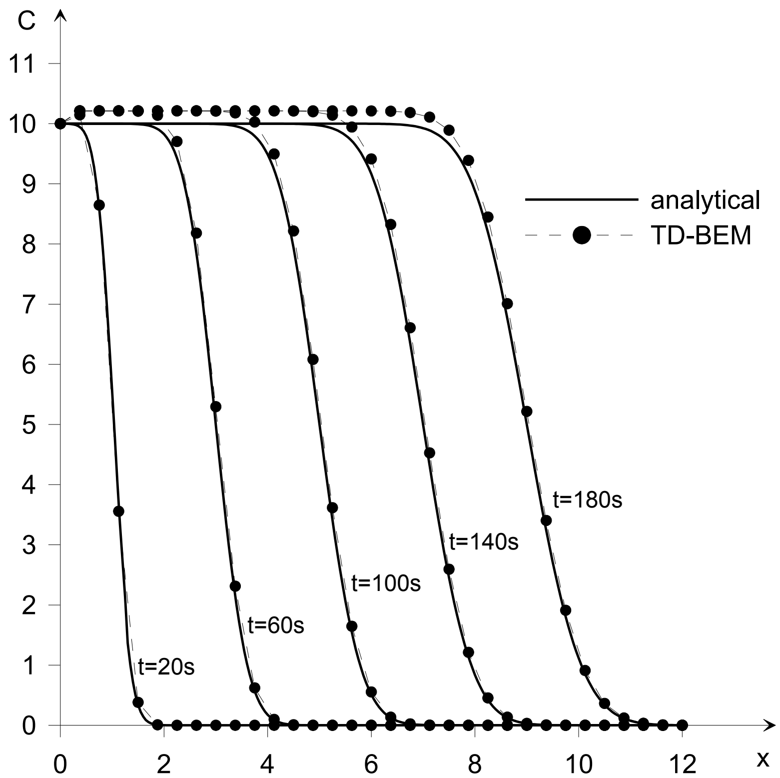

Figure 4: Results for $Pe = 10$.

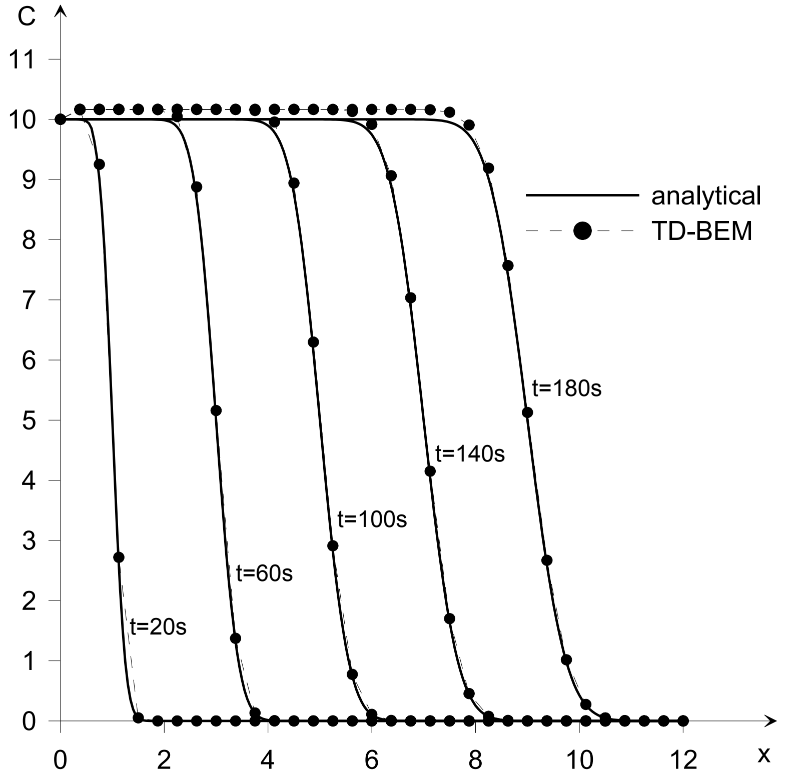

Figure 5: Results for $Pe = 20$.

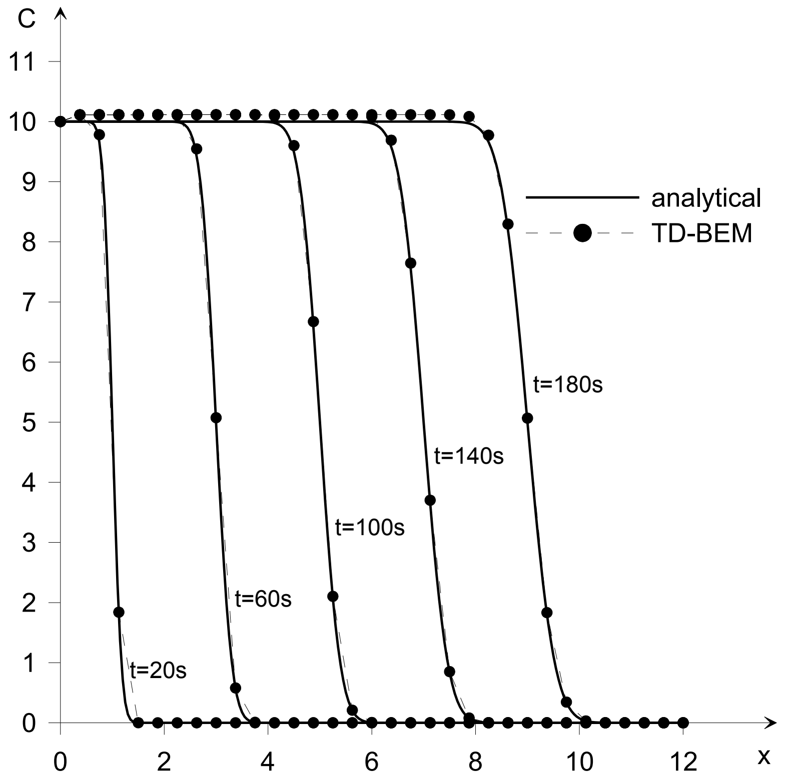

Figure 6: Results for Pe = 40.

With respect to the results presented in Fig. (3) to (6), one can note that the TD-BEM results present no artificial diffusion and oscillatory behavior, as observed in the D-BEM formulation presented by Taigbenu and Liggett (1986). Unfortunately, the TD-BEM results present overshooting, which increases from $Pe = 5$ (see Fig. (3)) to $Pe = 10$ (see Fig. (4)), as expected, but decreases from $Pe = 10$ to $Pe = 40$. It is the authors' reasoning that this unusual feature is difficult to explain based on a simple example. On the other hand, this feature is very favourable and can stimulate, even more, BEM studies in this promising area of research.

The L_2 norm

$$L_2 = \left[\frac{\sum_{m=1}^{N} (u_{i,exact} - u_{i,numer})^2}{\sum_{m=1}^{N} u_{i,exact}} \right]^{\frac{1}{2}}, \tag{16}$$

where $u_{i,exact}$ is the analytical solution, $u_{i,numer}$ is the numerical solution and N is the total number of points, was computed for each analysis, Pe number and selected time. The results are summarized in Fig. (7). One can verify that low L_2 norm values were achieved, what means that the BEM results are quite good.

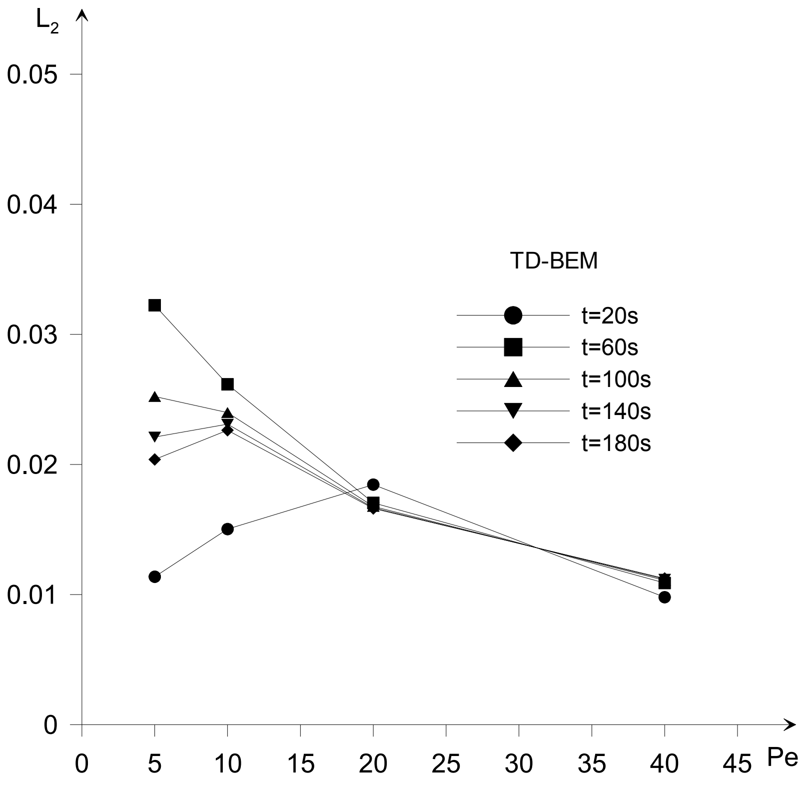

Figure 7: L_2 norm.

5 CONCLUSIONS

The development of the a TD-BEM formulation is always a challenge that stimulates the research work, due to the inherent difficulties that arise when time-dependent fundamental solutions are employed. The success of the TD-BEM formulation, relative success as this conclusion is based only on the good results presented here, is transitory and points to the improvement of the formulations, always aiming at the solution of more realistic problems. The search for adequate fundamental solutions turns time-domain formulations more difficult to cope with, but the elegance of the formulation and the accuracy of the results it produces, plenty justifies facing this challenge.

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