Anomalous diffusion equation modeled by the joint use of domain boundary element method and analytical derived solution based on green equation

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Abstract. In some situations, the mathematical formulation of the diffusion phenomenon might be described through a differential equation, which takes into account complementary and different effects with respect to the physical processes simulated with the support of the Fick´s equation, which is usually adopted to represent the diffusion process. In particular, diffusion applied to spatial-temporal retention problems with bimodal mass transmission is highlighted. To better understand this physical phenomenon, the proper use of the analytical Green function (GF) was investigated. The formulation employs the steady-state fundamental solution. In addition to the basic integral equation, another one is required, due to the fourth-order differential operator introduced in the differential equation of the problem evaluated. The domain discretization employs linear cells. The first order time derivative is approximated by a backward finite difference scheme. Two examples are presented. Numerical results are compared with analytical solutions showing good agreement between them; such framework provides a novel perspective for the use of the combined approach here developed to assess the behavior of physical phenomena better described by the fourth order analytical equation based on Green Function. In this work, the Domain Boundary Element Method (D-BEM) is explored to model that anomalous diffusion process taking into consideration that we were also able to originally develop the Green analytical solutions for the fourth order diffusion equation. Such combination of approaches proves to establish a new conceptual reference in this area.

Keywords: Anomalous Diffusion Equation, bimodal mass transmission, Domain Boundary Element, Method analytical Green Function, linear cells and backward finite difference scheme.

1 Introduction

Several mathematical formulations have been proposed to study different processes of mass transport, which consider in the physical systems the phenomenon of diffusion added to the effects of temporal retention [1], [2], [3], [4], [5] and [6]. Other works showed that the diffusion process applied to the problems of bimodal mass transmission have to considere the effects spatial-temporal retention. This physical process is sometimes referred to as the fourth order diffusion equation or anomalous diffusion process, previously presented by [7], [8] and [9].

In this work, the Domain Boundary Element Method (D-BEM) is explored to model that anomalous diffusion process taking into consideration the Green analytical solutions for the fourth order diffusion equation (see [10] and [11]). Such a combination of approaches proves to establish a new conceptual reference in this area. In fact, under the knowledge of the authors, this paradigmatic step, as we believe to be, is the first attempt ever made to solve the problem by means of the BEM implemented based on our original derived analytical solutions. In this paper, we address 1-D problems for showing the successful results achieved. Given this framework, it can be said that, once a fundamental solution corresponding to the steady state problem was obtained, a D-BEM type formulation was then developed. As it is well-known, such kind of formulations present a full domain whose integrand is, for the problem at hand, the fundamental solution multiplied by the first order time derivative of the variable of interest, or variable of the problem [12].

As the problem presents two natural boundary conditions, which are made up of the derivatives of order two and three of the problem variable, and two essential boundary conditions, namely the problem variable and its first order derivative, the basic BEM integral equation alone is not sufficient for providing the solution of the problem. In this way, similarly to what has been done to the problem of flexural analysis of beams [13], another BEM equation turns to be necessary. Such equation is that related to the first order derivative of the problem variable, and it is obtained by taking the derivative of the basic BEM equation with respect to the source point coordinate. Thus, a set of two integral equations is obtained and the problem can be solved appropriately. The domain integrals that remain in the system of equations are computed through domain discretization. Such a discretization employs linear cells, over which the first order time derivative of the variable of interest is assumed to vary linearly. The time-marching, by its turn, is carried out by simply employing a backward finite-difference scheme [14].

2 The Anomalous Diffusion Equation

The anomalous diffusion equation, as presented by [7], reads:

$$\beta D \frac{\partial^2 v(x,t)}{\partial x^2} - (1-\beta)\beta R \frac{\partial^4 v(x,t)}{\partial x^4} = \frac{\partial v(x,t)}{\partial t} \tag{1}$$

Equation (1) was obtained by considering a bi-modal flux distribution for the diffusion process associated with two energy states. The parameter β indicates the fraction of the particles in the main energy state, and the parameter R controls the effect of the secondary flux. Complementarily, D is the usual diffusion coefficient. The fourth order term with negative sign introduces the effect of retention. When, in Equation (1), β equals 1, one obtains the classical diffusion equation for isotropic media. It should be noticed that similar equations could be obtained by introducing non-linear effectson the Fick's Law see [3]. The boundary conditions, at x = 0 or at x = L, are:

i) Dirichlet type

$$v(x,t) = \underline{v}(x,t) \tag{2}$$

$$\frac{\partial v(x,t)}{\partial x} = \underline{v}'(x,t) \tag{3}$$

ii) Neumann type

$$\frac{\partial^2 v(x,t)}{\partial x^2} = \underline{v}''(x,t) \tag{4}$$

$$\frac{\partial^3 v(x,t)}{\partial x^3} = \underline{v}'''(x,t) \tag{5}$$

The initial condition for the interval $0 \leq x \leq L$is:

$$v(x,0) = v_0 \tag{6}$$

2.1 BEM formulation

A residual statement (see [14] and [15]), can be applied to Equation (1), with the fundamental solution of the steady-state problem playing the role of the weighting function. The following equation arises:

$$\begin{aligned} v(\varepsilon) = & -\sqrt{(1-\beta)R\beta}\,[v^*(\varepsilon,x)v'''(x)]_{x=0}^{x=L} + \sqrt{(1-\beta)R\beta}\left[\frac{\partial\, v^*(\varepsilon,x)}{\partial x}v''(x)\right]_{x=0}^{x=L} \\ & -\left[(\sqrt{(1-\beta)R\beta}\,\frac{\partial^2\, v^*(\varepsilon,x)}{\partial x^2} - \beta D v^*(\varepsilon,x))v'(x)\right]_{x=0}^{x=L} \\ & +\left[(\sqrt{(1-\beta)R\beta}\,\frac{\partial^3\, v^*(\varepsilon,x)}{\partial x^3} - \beta D\,\frac{\partial\, v^*(\varepsilon,x)}{\partial x})v(x)\right]_{x=0}^{x=L} \\ & -\int_0^{\varepsilon} \dot{v}(x,t)\, v^*(\varepsilon,x)dx - \int_{\varepsilon}^{L} \dot{v}(x,t)\, v^*(\varepsilon,x)dx \end{aligned} \tag{7}$$

The fundamental solution of the steady-state problem, $v^* = v^*(\varepsilon,x)$, is the solution ofEquation (1) (see [10, 11]) that can be written as

$$v^*(\varepsilon,x) = \left[\frac{\sqrt{(1-\beta)R\beta}\left(sinh\left[\sqrt{\frac{\beta D}{(1-\beta)R\beta}}r\right]\right) + \sqrt{\beta D}\, r}{2(\beta D)^{\frac{3}{2}}}\right] \tag{8}$$

where $r = |x-\varepsilon|$ is the distance between field, x, and source, ε, points. As previously mentioned in the introductory section of this work, Equation (7) alone is not sufficient to provide the solution of the problem. Another equation becomes necessary.
This equation is obtained by taking the derivative of Equation (7) with respect to the source point coordinate, and reads:

$$\frac{\partial v(\varepsilon)}{\partial \varepsilon} = -\sqrt{(1-\beta)R\beta}\left[\frac{\partial v^*(\varepsilon,x)}{\partial \varepsilon} v'''(x)\right]_{x=0}^{x=L} + \sqrt{(1-\beta)R\beta}\left[\frac{\partial^2 v^*(\varepsilon,x)}{\partial \varepsilon \partial x} v''(x)\right]_{x=0}^{x=L}$$
$$- \left[(\sqrt{(1-\beta)R\beta}\,\frac{\partial^3 v^*(\varepsilon,x)}{\partial \varepsilon \partial x^2} - \beta D \frac{\partial v^*(\varepsilon,x)}{\partial \varepsilon}) v'(x)\right]_{x=0}^{x=L}$$
$$+ \left[(\sqrt{(1-\beta)R\beta}\,\frac{\partial^4 v^*(\varepsilon,x)}{\partial \varepsilon \partial x^3} - \beta D \frac{\partial^2 v^*(\varepsilon,x)}{\partial x \partial \varepsilon}) v(x)\right]_{x=0}^{x=L} \tag{9}$$
$$- \int_0^{\varepsilon} \dot{v}(x,t) \frac{\partial v^*(\varepsilon,x)}{\partial \varepsilon} dx - \int_{\varepsilon}^{L} \dot{v}(x,t) \frac{\partial v^*(\varepsilon,x)}{\partial \varepsilon} dx$$

The derivatives that appear in Equations (7) and (17) are computed. One has, in a simplified notation, the following:

$$\frac{\partial v^*(\varepsilon,x)}{\partial x} = \frac{-1}{2\beta D}\left(cosh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r + 1\right)\frac{\partial r}{\partial x} \tag{10}$$

$$\frac{\partial^2 v^*(\varepsilon,x)}{\partial x^2} = \frac{-1}{2\sqrt{\beta^2 D(1-\beta)R}}\left(sinh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r\right)\left(\frac{\partial r}{\partial x}\right)^2 \tag{11}$$

$$\frac{\partial^3 v^*(\varepsilon,x)}{\partial x^3} = \frac{-1}{2\sqrt{(1-\beta)R\beta}}\left(cosh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r\right)\left(\frac{\partial r}{\partial x}\right)^3 \tag{12}$$

And from equation (9), one has:

$$\frac{\partial v^*(\varepsilon,x)}{\partial \varepsilon} = \frac{-1}{2\beta D}\left(cosh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r + 1\right)\frac{\partial r}{\partial \varepsilon} \tag{13}$$

$$\frac{\partial^2 v^*(\varepsilon,x)}{\partial \varepsilon \partial x} = \frac{-1}{2\sqrt{\beta^2 D(1-\beta)R}}\left(sinh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r\right)\frac{\partial r}{\partial x}\frac{\partial r}{\partial \varepsilon} \tag{14}$$

$$\frac{\partial^3 v^*(\varepsilon,x)}{\partial \varepsilon \partial x^2} = \frac{-1}{2\sqrt{\beta(1-\beta)R}}\left(cosh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r\right)\left(\frac{\partial r}{\partial x}\right)^2\frac{\partial r}{\partial \varepsilon} \tag{15}$$

$$\frac{\partial^4 v^*(\varepsilon,x)}{\partial \varepsilon \partial x^3} = \frac{-\sqrt{\beta D}}{2(\beta(1-\beta)R)^{\frac{3}{2}}}\left(sinh\sqrt{\frac{\beta D}{(1-\beta)R\beta}}\, r\right)\left(\frac{\partial r}{\partial x}\right)^3\frac{\partial r}{\partial \varepsilon} \tag{16}$$

The domain discretization is necessary due to the domain integrals indicated in Equations (7) and (9). In this work, linear cells weread opted, i.e. $\dot{v}(x,t)$ varies linearly inside each cell. Analytical integration is easily carried out. For this reason, further details are omitted here. Finally, the last required approximation is related to $\dot{v}(x,t)$. The time derivative is approximated by adopting a backward finite difference. For a given time, say $t_{n+1} = (n+1)\Delta t$, where Δt is the time-step, one has:

$$\dot{v}(x,t_{n+1}) = \dot{v}_{n+1} = \frac{v_{n+1} - v_n}{\Delta t} \qquad n = 0, 1, 2, 3 \ldots \tag{17}$$

To solve the problem, Equations (7) and (9) are written, or particularized, for $\varepsilon = 0$ and for $\varepsilon = L$, and the domain integrals are computed. The next step is to replace, in Equation (7), the derivatives given in Equations (10), (11) and (12). In the absence of studies concerning the choice of the time-step length, it was chosen empirically. For some recommend ations concerning its choice, the reader is referred to [11]. In matrix form, the system of algebraic equations can be written as:

$$\begin{bmatrix} (\Delta t\mathbf{H}^{bb}+\mathbf{W}^{bb}) & -\Delta t\boldsymbol{v}^{bb} & (0+\mathbf{W}^{bd}) \\ (0+\overline{\mathbf{W}}^{bb}) & \Delta t\boldsymbol{v}^{bb} & (0+\overline{\mathbf{W}}^{bd}) \\ (-\Delta t\mathbf{H}^{db}+\mathbf{W}^{db}) & -\Delta t\boldsymbol{v}^{db} & (\Delta tI+\mathbf{W}^{dd}) \end{bmatrix} \begin{Bmatrix} v_{n+1}^{b} \\ v'^{b}_{n+1} \\ v_{n+1}^{d} \end{Bmatrix} = \begin{bmatrix} \Delta t\mathbf{G}^{bb} & \Delta t\boldsymbol{B}^{bb} \\ \Delta t\overline{\mathbf{G}}^{bb} & \Delta t\overline{\mathbf{B}}^{bb} \\ \Delta t\mathbf{G}^{db} & \Delta t\mathbf{B}^{db} \end{bmatrix} \begin{Bmatrix} v'''^{b}_{n+1} \\ v''^{b}_{n+1} \end{Bmatrix} - \begin{bmatrix} \mathbf{D}^{bb} & 0 & \mathbf{W}^{bd} \\ \overline{\mathbf{D}}^{bb} & 0 & \overline{\mathbf{W}}^{bd} \\ \mathbf{D}^{db} & 0 & \mathbf{W}^{dd} \end{bmatrix} \begin{Bmatrix} 5v_n^{b} \\ 0 \\ v_n^{d} \end{Bmatrix} \quad (18)$$

The superscripts **b** and **d**, concerningthevectors in Equation (18), correspond to the boundary nodes and to the domain internal points, respectively. Then, vectors v_{n+1}^{b}, v'^{b}_{n+1},v''^{b}_{n+1} and v'''^{b}_{n+1} have dimension (2x1), where as vector v_{n+1}^{d}hasdimension (n_i), with n_i being the number of internal points. Note that the number of cells is equal to (n_i+1). The identity matrix I is related to the internal points. In the sub-matrices, the first super script corresponds to the position of the source point and the second to the position of the field point. Concisely, Equation (31) can be written as presented in [10]:

$$\bar{H}d_{n+1} = \bar{G}n_{n+1} + \bar{W}u_n \quad (19)$$

In Equation (19), the vector d_{n+1}contains the values of v and v', related to the essential boundary conditions, and the vector n_{n+1}contains the values of v'' and v''', related to the natural boundary conditions. Matrices $\bar{H}$ and $\bar{G}$ come from the expressions (7) – (9) and matrix $\bar{W}$ comes from the domainintegrations [10].

2.2 Numerical results DBEM

In the examples presented in this section, the following parameters were adopted:

D = 1
R = 0.05 and R = 0.5
β = 1

All the analyses were carried out with the domaind is discretized into 16 cells. The time-step length was:

Δt = 0.05s

This example consists of a domain of unity length, with all the boundary conditions null and with na initial condition field given by:

$$v(x,t) = v_0 cos\left(\frac{\pi}{2}x\right) \quad (20)$$

The analytical solution to this problem is given by (see[11]) as

$$v(x,t) = v_0 exp\left(\frac{\pi^2}{4}\ D\rho t\right) cos\ cos\left(\frac{\pi x}{2}\right) \quad (21)$$

with

$$\rho = -\beta\left(1 + \frac{\pi^2}{4}\frac{R}{D}(1-\beta)\right) \quad (22)$$

Figure 1 depicts the results at various values of "t" for the first analysis, carried out with $R = 0.05$, where as Figure 2 depicts the results for the second analysis, for which $R = 0.5$.

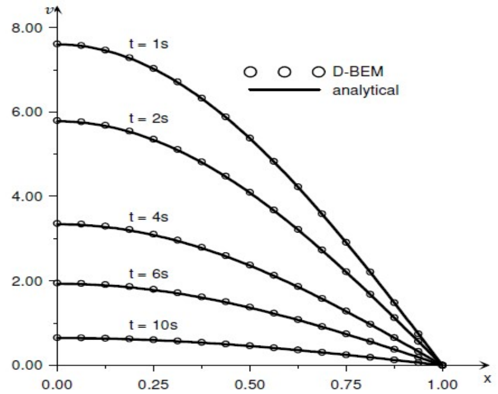

Figure 1. Example 1: results at different instants of time for $R = 0.05$.

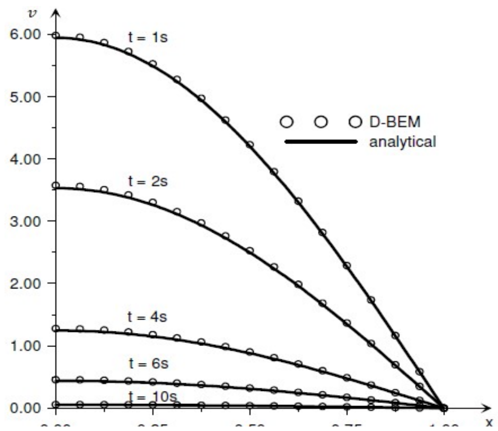

Figure 2. Example 1: results at different instants of time for $R = 0.5$.

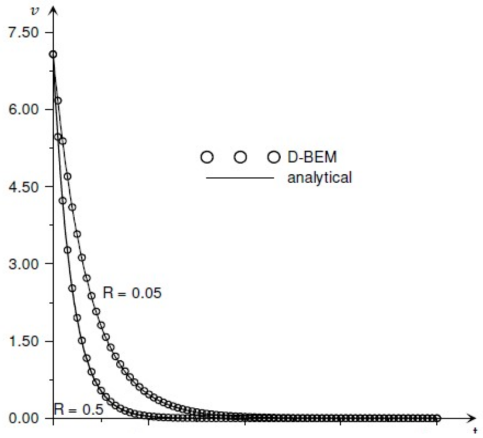

Figure 3. Example 1: results for $v(0.5, t)$.

Note that the ratio $\rho = \rho(r, \beta)$, defined by Equation (22), controls the rate of change of the variable of interest. When $\beta = 1$, the problem is reduced to the classical diffusion problem. Figure 3 depicts the results of the first and second analyses for $v(0.5, t)$. In all Figures, a good agreement is observed between the analytical solution and the BEM results.

3 Conclusions

This work is concerned with the solution of the anomalous diffusion equation, in one-dimension (1-D), by employing the BEM. Although one-dimensional problems present a limited range of applications, their solutions always give there searcher experience for facing more complex problems in two and three dimensions. For the problem treated here, a fundamental solution, associated to the steady state problem, was found and a successful D-BEM formulation was developed. The results generated by the formulation are accurate and present good agreement with analytical solutions. Naturally, this is the first step to wards the development of new BEM formulations. The search for a time-dependent fundamental solution, at this time, seems to be very challenging, as well as the development of formulations for bi- and three-dimensional problems. Another problem that should deserve attention is the one to deal with anisotropic materials.

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