Engineering Analysis with Boundary Elements 65 (2016) 79–94

Contents lists available at ScienceDirect

Engineering Analysis with Boundary Elements

journal homepage: www.elsevier.com/locate/enganabound

A study concerning the solution of advection–diffusion problems by the Boundary Element Method

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ARTICLE INFO

Article history:
Received 31 October 2014
Received in revised form
15 December 2015
Accepted 4 January 2016
Available online 25 January 2016

Keywords:
Boundary Element Method
Finite Element Method
Advection–diffusion equation
FEM
D-BEM
TD-BEM

ABSTRACT

This work is concerned with the development of two Boundary Element Method formulations for the solution of the advection–diffusion problem in two-dimensions. Beside the discussion concerning the development of the BEM formulations, 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 formulations capable of dealing with this social and environmental problem is welcome. In order to verify the accuracy of the proposed formulations, two examples are presented. The numerical results are compared with the analytical solution, when available, and with the results from the Finite Element Method.

1. Introduction

The advection–diffusion equation describes an actual 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. The analytical solutions, however, are usually developed for profiles with known form and, consequently, this simplification results in loss of quality for some dispersion problems in real situations. Among others, Kumar et al. [1] analyzed the analytical solution for one-dimensional advection–diffusion equation with variable coefficients in semi-infinite domain, using Laplace transformation technique and Yadav et al. [2] also presented analytical solutions for several boundary conditions.

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 works can be cited: the FEM and FDM formulations, for the two-dimensional equation, are presented in Zhao et al. [3]; Ataie-Ashtiani and Hosseini [4] employed the FDM with different schemes and presented a study concerning their stability; Prieto et al. [5] presented the solution of tri-dimensional advection–diffusion equation by explicit FDM formulations, devoting special attention to the criterion of stability and, in Dhawan et al. [6], the solution for one-dimensional advection–diffusion equation, with B-spline FEM, is compared with the analytical solution.

With the purpose of contributing with the discussion concerning the solution of the advection–diffusion equation, two Boundary Element Method (BEM) formulations are presented in this paper. For the academic point of view, the development of different formulations of the same method enriches the discussion concerning the possibilities of the method and enlarges its range of applications. For general purposes, however, the use of the BEM as a tool for the solution of the advection–diffusion equation is the main contribution of the paper. Different BEM formulations arise according to the fundamental solution employed in obtaining the basic integral equation of the method, see Polyanin [7] 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: TD-BEM, TD meaning time-domain; D-BEM, D meaning domain and DR-BEM, DR meaning dual reciprocity. A brief outline of the formulations follows in the sequence. The TD-BEM formulation employs time-dependent fundamental solutions. As a consequence, the solution of problems with homogeneous initial conditions requires only the boundary discretization, whereas the presence of non-homogeneous initial conditions requires only the discretization of the part of the domain where it occurs, e.g. Wrobel [8] and Young et al.

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http://dx.doi.org/10.1016/j.enganabound.2016.01.002
0955-7997/

[9]. Very elegant from the mathematical point of view and provider of accurate results, the main criticism for the TD-BEM formulation is the high computational cost involved in the assemblage of the matrices. 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 [10]. If the domain integral is kept in the integral equation, then the D-BEM arises, e.g. Taigbenu and Liggett [11], Carrer et al. [12], Carrer and Mansur [13], and Pettres et al. [14]. 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. Regarding the D-BEM formulation presented in this work, the choice is the simplest one, that is, a backward finite difference scheme is adopted, Smith [15]. Before finishing this brief discussion, it is important to mention that attention has been devoted to meshless approaches; see for instance Boztosun and Charafi [16], Bourantas et al. [17], and Bourantas and Burganos [18]. Another promising area of research that also deserves be mentioned is that related to isogeometric boundary element methods. Several articles appeared in the literature recently, e.g. Simpson et al. [19,20] and Schillinger et al. [21].

The comparison between the BEM and FEM results enables verifying the accuracy provided by both BEM formulations. The FEM formulation is included for completeness purpose, aiming at enriching the content of the paper. Two examples are included. The first one is the already classic one-dimensional transport problem in a semi-infinite medium, which has an analytical solution, see Ogata and Banks [22]. The BEM results are compared with the analytical solution and with the FEM results for problems with high Peclet numbers, enabling one to assess the potentialities of the D-BEM and the TD-BEM formulations. The second example consists of a two-dimensional transport problem with initial conditions in a part of the domain. In the absence of an analytical solution, the FEM results are treated as the reference ones.

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:

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

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, D is the diffusion coefficient and K represents the first-order decay constant.

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:

$$U_nC-D\frac{dC}{dn}=F_n^* \tag{2}$$

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

$$U_nC=F_n^* \tag{4}$$

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 $\Gamma=\Gamma_Q\cup\Gamma_C$.

The initial conditions, over the domain Ω, are:

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

3. Numerical models

As mentioned at the Introduction to this work, two Boundary Element Method (BEM) formulations were developed for the solution of Eq. (1). A FEM model was also employed, with the aim of validating the BEM results. This section starts presenting the BEM formulations and finishes with the presentation of the FEM formulation. A brief discussion follows each formulation, together with the recommended references for additional details.

3.1. BEM formulations

By following a procedure based on the method of the weighting residuals, see, for instance, the textbooks by Brebbia et al. [23], Zienkiewicz and Morgan [24], Brebbia and Connor [25], and Finlayson [26], the BEM formulations differ according to the fundamental solution, Polyanin [7], employed as the weighting function. Here, the first formulation employs the fundamental solution associated with the steady-state problem; consequently, it is a not time-dependent one. As a consequence, a domain integral containing the first order time derivative of the substance concentration appears in the BEM integral equation and, for the numerical analysis, the entire domain discretization is required. For this reason, this formulation is referred to as D-BEM, with D meaning domain. According to the authors' reasoning, the main characteristic of the BEM is the use of fundamental solutions as weighting functions, all formulations which satisfy this requirement being a BEM one. In this way, the notation with the D letter is employed in this paper only because of the tradition in its use and to differentiate this formulation from the second one, which employs a time-dependent fundamental solution. This formulation is referred to as TD-BEM, TD meaning time-domain. For the numerical analysis, only the boundary is discretized in problems without initial conditions. The presence of initial conditions, on the other hand, requires the discretization only of the part of the domain where they occur, see the second example.

Before presenting the BEM formulations, a brief account is given concerning the boundary and the domain discretization. The boundary discretization employs linear elements. The domain discretization employs triangular linear cells. The interested