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A novel dual reciprocity boundary element formulation for two-dimensional transient convection–diffusion–reaction problems with variable velocity

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ABSTRACT

This paper describes a new formulation of the dual reciprocity boundary element method (DRBEM) for two-dimensional transient convection–diffusion–reaction problems with variable velocity. The formulation decomposes the velocity field into an average and a perturbation part, with the latter being treated using a dual reciprocity approximation to convert the domain integrals arising in the boundary element formulation into equivalent boundary integrals. The integral representation formula for the convection–diffusion–reaction problem with variable velocity is obtained from the Green's second identity, using the fundamental solution of the corresponding steady-state equation with constant coefficients. A finite difference method (FDM) is used to simulate the time evolution procedure for solving the resulting system of equations. Numerical applications are included for three different benchmark examples for which analytical solutions are available, to establish the validity of the proposed approach and to demonstrate its efficiency. Finally, results obtained show that the DRBEM results are in excellent agreement with the analytical solutions and do not present oscillations or damping of the wave front, as it appears in other numerical techniques.

1. Introduction

The solution of convection–diffusion–reaction problems is a difficult task for all numerical methods because of the nature of the governing equation, which includes first-order and second-order partial derivatives in space [1–5]. The convection–diffusion equation is the basis of many physical and chemical phenomena, and its use has also spread in economics, financial forecasting and other fields [6]. The dual reciprocity boundary element method (DRBEM), initially applied to transient heat conduction problems by Wrobel et al. [7], interprets the time derivative in the diffusion equation as a body force and employs the fundamental solution to the corresponding steady-state equation to generate a boundary integral equation. When the steady-state fundamental solution is used in the DRBEM to approximate transient convection–diffusion problems, other techniques should be employed to approximate the solution's functional dependence on the temporal variables. Aral and Tang [8] used the fundamental solution of the Laplace equation, but made use of a secondary reduction process, called SR-BEM, to arrive at a boundary-only formulation. They presented the results of transient convection–diffusion problems with or without first order chemical reaction for low to moderate Péclet numbers. Martin [9] proposed a Schwartz waveform relaxation algorithm for the unsteady diffusive–convective equation, which uses domain decomposition methods and applies the iterative algorithm directly to the time-dependent problem. Partridge and Sensale [10] have used the method of fundamental solution with dual reciprocity and subdomain approach to solve convection–diffusion problems. The time integration scheme is the finite difference method (FDM) with a relaxation procedure, which is iterative in nature and needs a carefully selected time increment. Regarding the DRBEM formulation presented in this work, a backward finite difference scheme is adopted, Smith [11].

In this article, the DRBEM is also employed to discretise the spatial partial derivatives in the two-dimensional diffusive–convective–reactive type problem. Thus, the problem is ultimately described in terms of boundary values only, consequently reducing its dimensionality by one [12]. We use the fundamental solution to the steady-state convection–diffusion–reaction equation and transform the domain integral arising from the time derivative term using a set of coordinate functions and particular solutions which satisfy the associated non-homogeneous steady-state convection–diffusion–reaction problem. Further, only a simple set of cubic radial basis functions has been previously used in this formulation. We consider two other sets of coordinate func-

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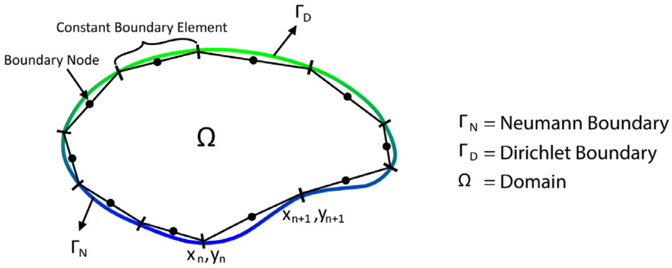

Fig. 1. Definition of domain, boundary, and constant elements.

tions, non-augmented thin plate splines (TPS) and multiquadric (MQ) radial basis functions, and analyse their performance in conjunction with order of time integration algorithms for convection–diffusion–reaction problems. This work also focuses on the search for the optimal shape parameter when utilising the multiquadric radial basis function (MQ-RBF). This is due to the lack of information on choosing the best shape parameter, forcing the user having to make an 'ad-hoc' decision. Recent numerical experiments available in the literature, nevertheless, showed that the MQ-RBF has shown great potential when dealing with complicated PDEs in two dimensions if an adequate shape value is provided.

A brief outline of the rest of this paper is as follows. Section 2 reviews the representation of convection–diffusion–reaction. Section 3 derives the boundary element formulation of the governing equation using the steady-state fundamental solution of the corresponding equation. In Sections 4 and 5, the DRBEM formulation and its discretisation are developed for the 2D transient convection–diffusion–reaction problem. A two-level time marching procedure for the proposed model is implemented in Section 6. Section 7 gives the description of the coordinate functions and the choice of the three radial basis functions. Section 8 compares and investigates the solution profiles for the present numerical experiments with the analytical solution of the tested cases. Computational aspects are included to demonstrate the performance of the approach in Section 9. Finally, some conclusions and remarks are provided in the last section.

2. Convection–diffusion–reaction equation

The two dimensional transient convection–diffusion–reaction problem over a domain Ω in $\mathbb{R}^2$ bounded by a boundary Γ, for isotropic materials, is governed by the following PDE:

$$D\nabla^2\phi(x,y) - \upsilon_x(x,y)\frac{\partial\phi(x,y)}{\partial x} - \upsilon_y(x,y)\frac{\partial\phi(x,y)}{\partial y} - k\,\phi(x,y) = \frac{\partial\phi(x,y)}{\partial t},\quad (x,y)\in\Omega,\ t>0 \tag{1}$$

In Eq. (1), ϕ represents the concentration of a substance, treated as a function of space and time. The velocity components v_x and v_y along the x and y directions and assumed to vary in space. Besides, D is the diffusivity coefficient and k represents the first-order reaction constant or adsorption coefficient. The boundary conditions are

$$\phi = \bar{\phi} \quad \text{over} \quad \Gamma_D \tag{2}$$

$$q = \frac{\partial\phi}{\partial n} = \bar{q} \quad \text{over} \quad \Gamma_N, \tag{3}$$

where Γ_D and Γ_N are the Dirichlet and Neumann parts of the boundary with $\Gamma = \Gamma_D \cup \Gamma_N$, and $\Gamma_D \cap \Gamma_N = 0$ (see Fig. 1). The initial condition over the domain Ω is

$$\phi(x,y,t=0) = \phi_0(x,y),\quad (x,y)\in\Omega \tag{4}$$

The parameter that describes the relative influence of the convective and diffusive components is called the Péclet number, $\text{Pé} = |\upsilon|L/D$, where $\upsilon = \left(\upsilon_x^2+\upsilon_y^2\right)^{1/2}$ is the velocity field and L is a characteristic length of the domain. For small values of Pé, Eq. (1) behaves as a parabolic differential equation in time, while for large values the equation becomes more like hyperbolic. These changes in the structure of the PDE according to the values of the Péclet number have significant effects on its numerical solution.

3. Boundary element formulation of transient convection–diffusion–reaction problems using steady-state fundamental solution

Let us consider a region $\Omega \subset \mathbb{R}^2$ bounded by a piecewise smooth boundary Γ. The transport of ϕ in the presence of a reaction term is governed by the two-dimensional transient convection–diffusion–reaction Eq. (1). The variable ϕ can be interpreted as temperature for heat transfer problems, concentration for dispersion problems, etc., and will be herein referred to as a potential. For the sake of obtaining an integral equation equivalent to the above PDE, a fundamental solution of Eq. (1) is necessary. However, fundamental solutions are only available for the case of constant velocity fields. At this stage, the variable velocity components $\upsilon_x = \upsilon_x(x,y)$ and $\upsilon_y = \upsilon_y(x,y)$ are decomposed into average (constant) terms $\bar{\upsilon}_x$ and $\bar{\upsilon}_y$, and perturbations $P_x = P_x(x,y)$ and $P_y = P_y(x,y)$, such that

$$\upsilon_x(x,y) = \bar{\upsilon}_x + P_x(x,y),\quad \upsilon_y(x,y) = \bar{\upsilon}_y + P_y(x,y) \tag{5}$$

Now, we can re-write Eq. (1) to take the form

$$D\nabla^2\phi(x,y) - \bar{\upsilon}_x(x,y)\frac{\partial\phi(x,y)}{\partial x} - \bar{\upsilon}_y(x,y)\frac{\partial\phi(x,y)}{\partial y} - k\,\phi(x,y) = \frac{\partial\phi(x,y)}{\partial t} + P_x\frac{\partial\phi(x,y)}{\partial x} + P_y\frac{\partial\phi(x,y)}{\partial y}. \tag{6}$$

Next, one can transform the differential Eq. (6) into an equivalent integral equation as follows [12]:

$$\phi(\xi) - D\int_\Gamma \phi^*\frac{\partial\phi}{\partial n}\,d\Gamma + D\int_\Gamma \phi\,\frac{\partial\phi^*}{\partial n}\,d\Gamma + \int_\Gamma \phi\,\phi^*\,\bar{\upsilon}_n\,d\Gamma = -\int_\Omega\left[\frac{\partial\phi}{\partial t} + \left(P_x\frac{\partial\phi}{\partial x} + P_y\frac{\partial\phi}{\partial y}\right)\right]\phi^*\,d\Omega,\ \xi\in\Omega \tag{7}$$

where $\bar{\upsilon}_n = \upsilon.n$, n is the unit outward normal vector and the dot stands for scalar product and $\upsilon = \left(\upsilon_x, \upsilon_y\right)$. In the above equation, ϕ^* is the fundamental solution of the steady-state convection–diffusion–reaction equation with constant coefficients. For two-dimensional problems, ϕ^* is given by

$$\phi^*(\xi,\chi) = \frac{1}{2\pi D}\,e^{-\left(\frac{\bar{\upsilon}.r}{2D}\right)}K_0(\mu r), \tag{8}$$

where

$$\mu = \left[\left(\frac{|\bar{\upsilon}|}{2D}\right)^2 + \frac{k}{D}\right]^{\frac{1}{2}},\quad \bar{\upsilon} = \left(\bar{\upsilon}_x, \bar{\upsilon}_y\right) \tag{9}$$

in which ξ and χ are the source and field points, respectively, and r is the modulus of $\mathbf{r} = |\chi - \xi|$, the distance vector between the source and field points. The derivative of the fundamental solution with respect to the outward normal is given by

$$\frac{\partial\phi^*}{\partial n} = \frac{1}{2\pi D}\,e^{-\left(\frac{\bar{\upsilon}.r}{2D}\right)}\left[-\mu\,K_1(\mu r)\,\frac{\partial r}{\partial n} - \frac{\bar{\upsilon}_n}{2D}\,K_0(\mu r)\right] \tag{10}$$

In the above, K_0 and K_1 are Bessel functions of second kind, of orders zero and one, respectively. The exponential term is responsible for the inclusion of the correct amount of 'upwind' into the formulation [13]. Eq. (7) is valid for source points ξ inside the domain Ω. A similar expression can be obtained, by implementing Green's second identity and