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The dual reciprocity boundary element formulation for convection-diffusion-reaction problems with variable velocity field using different radial basis functions

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ABSTRACT

This paper presents a dual reciprocity boundary element method (DRBEM) formulation for the solution of steady-state convection-diffusion-reaction problems with variable velocity field at moderately high Péclet number. This scheme is based on utilising the fundamental solution of the convection-diffusion-reaction equation with constant coefficients. In this case, we decompose the velocity field into an average and a perturbation, 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. A proposed approach is implemented to treat the convective terms with variable velocity, for which the concentration is expanded as a series of functions. Four numerical experiments are included with available analytical solutions, to establish the validity of the approach and to demonstrate the efficiency of the proposed method.

1. Introduction

The boundary element method (BEM) has been applied to steady-state convection-diffusion-reaction problems with variable velocity by various researchers [1–9]. However, the solution of this problem is still considered a big challenge, particularly for variable and high velocities. The BEM does have an inherent advantage for the solution of convection-diffusion-reaction problems with constant velocity as the existing fundamental solution of the problem introduces the exact amount of upwind, contrary to finite element or finite-difference methods where the upwind is numerical [7]. The dual reciprocity boundary element method (DRBEM) represents an alternative for solving linear PDEs with variable coefficients [10–14]. The solution of problems involving variable coefficients is more difficult to achieve with the BEM as fundamental solutions are only available for a small number of cases, for coefficients with very simple variations in space. The approach adopted in this paper is to split the velocity field into an average and a perturbation; the average velocity (constant) is included in the fundamental solution, while the perturbation generates a domain integral which is treated with the DRBEM. A new particular solution has been used with corresponding dual reciprocity expressions. A proposed approach was implemented to treat the convective terms with variable velocity. Results of four test cases are presented and compared to analytical solutions. They show that the boundary element formulation developed in this work produces accurate results for diffusion-dominated problems with low velocity values.

A brief outline of the rest of this paper is as follows. Section 2 reviews the representation of convection-diffusion-reaction problems. Section 3 derives the boundary element formulation using the steady-state fundamental solution of the corresponding equation. In Section 4, the DRM formulation is developed for 2D steady-state convection-diffusion-reaction problem, followed in Section 5 by a description of the discretisation of the DRBEM formulation for this model. Handling the convective terms by expanding the relevant functions as a series are shown in Section 6. Section 7 gives the description of the coordinate functions and the three radial basis functions adopted in this work. Section 8 compares and discusses the solution profiles for the present numerical experiments. Computational aspects are included to demonstrate the performance of this approach in Section 9. Finally, some conclusions are provided in the last section.

2. Convection-diffusion-reaction equation

The two-dimensional convection-diffusion-reaction problem over a domain Ω in $\Re^2$ limited by a boundary Γ, for isotropic materials, is governed by the following PDE:

$$D\nabla^2\phi(x,y) - v_x(x,y)\frac{\partial\phi(x,y)}{\partial x} - v_y(x,y)\frac{\partial\phi(x,y)}{\partial y} - k\,\phi(x,y) = 0 \tag{1}$$

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$x, y \in \Omega \subset \Re^d, t > 0$

In Eq. (1), ϕ represents the concentration of a substance, treated as a function of space, Γ is a bounded domain in $\Re^d$, d is the dimension of the problem. 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 $\Gamma = \Gamma_D \cup \Gamma_N$.

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

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

For the sake of obtaining an integral equation equivalent to the above partial differential equation, a fundamental solution of Eq. (1) is necessary. However, fundamental solutions are only available for the case of constant velocity fields. Thus, 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

$$\upsilon_x(x, y) = \bar{\upsilon}_x + P_x(x, y)$$

$$\upsilon_y(x, y) = \bar{\upsilon}_y + P_y(x, y) \tag{4}$$

This permits rewriting Eq. (1) as

$$D\nabla^2 \phi - \bar{\upsilon}_x \frac{\partial \phi}{\partial x} - \bar{\upsilon}_y \frac{\partial \phi}{\partial y} - k\phi = P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y} \tag{5}$$

The above differential equation can now be transformed into the following equivalent integral equation

$$\phi(\xi) - D \int_\Gamma \phi^* \frac{\partial \phi}{\partial n} d\Gamma + D \int_\Gamma \phi \frac{\partial \phi^*}{\partial n} d\Gamma + \int_\Gamma \phi \phi^* \bar{\upsilon}_n d\Gamma = -\int_\Omega \left(P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y} \right) \phi^* d\Omega \tag{6}$$

where $\bar{\upsilon}_n = \bar{\upsilon}.n$, n is the unit outward normal vector and the dot stands for scalar product. In the above equation, ϕ^* is the fundamental solution of the convection-diffusion-reaction equation with constant coefficients. For two-dimensional problems, ϕ^* is of the form

$$\phi^*(\xi, \chi) = \frac{1}{2\pi D} e^{-\left(\frac{\bar{\upsilon}.r}{2D}\right)} K_0(\mu r) \tag{7}$$

where

$$\mu = \left[\left(\frac{\bar{\upsilon}}{2D} \right)^2 + \frac{k}{D} \right]^{\frac{1}{2}} \tag{8}$$

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

$$\frac{\partial \phi^*}{\partial n} = \frac{1}{2\pi D} e^{-\left(\frac{\bar{\upsilon}.r}{2D}\right)} \left[-\mu K_1(\mu r) \frac{\partial r}{\partial n} - \frac{\bar{\upsilon}_n}{2D} K_0(\mu r) \right] \tag{9}$$

In the above, K_0 and K_1 are Bessel functions of second kind, of orders zero and one, respectively (for more details of the fundamental solution and its normal derivative, see [4,6,10]). The exponential term is responsible for the inclusion of the correct amount of windinto the formulation [7]. Eq. (6) is valid for source points ξ inside the domain Ω. A similar expression can be obtained, by a limit analysis, for source points ξ on the boundary Γ, in the form

$$c(\xi)\phi(\xi) - D \int_\Gamma \phi^* \frac{\partial \phi}{\partial n} d\Gamma + D \int_\Gamma \phi \frac{\partial \phi^*}{\partial n} d\Gamma + \int_\Gamma \phi \phi^* \bar{\upsilon}_n d\Gamma = -\int_\Omega \left(P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y} \right) \phi^* d\Omega \tag{10}$$

in which $c(\xi)$ is a function of the internal angle the boundary Γ makes at point ξ.

4. DRM formulation for steady-state convection-diffusion-reaction problem

In the present formulation, we concentrate on the implementation of the dual reciprocity formulation DRM based on the fundamental solution to the steady-state convection-diffusion-reaction equation, where the convective velocity is assumed to be variable and is split into two parts, constant and perturbation, respectively. The basic idea is to expand the non-homogenous perturbation term on the right-hand side of Eq. (5) in the form

$$P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y} = \sum_{k=1}^{M} f_\alpha \alpha_k \tag{11}$$

This series contains a sequence of known functions $f_k = f_k(x, y)$, and a set of unknown coefficients α_k. Using this approximation, the domain integral in Eq. (10) can be approximated in the form

$$\int_\Omega \left(P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y} \right) \phi^* d\Omega = \sum_{k=1}^{M} \alpha_k \int_\Omega f_k \phi^* d\Omega \tag{12}$$

The next step is to consider that, for each function f_k, there exists a related function ψ_k which is a particular solution of the equation

$$D\nabla^2 \psi - \bar{\upsilon}_x \frac{\partial \psi}{\partial x} - \bar{\upsilon}_y \frac{\partial \psi}{\partial y} - k\psi = f \tag{13}$$

Thus, the domain integral can be recast in the form

$$\int_\Omega \left(P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y} \right) \phi^* d\Omega = \sum_{k=1}^{M} \alpha_k \int_\Omega \left(D\nabla^2 \psi_k - \bar{\upsilon}_x \frac{\partial \psi_k}{\partial x} - \bar{\upsilon}_y \frac{\partial \psi_k}{\partial y} - k\psi_k \right) \phi^* d\Omega \tag{14}$$

Substituting Eqs. (14) into (10), and utilising integration by parts in the domain integral of the resulting equation, we finally obtain a boundary integral equation of the form

$$c(\xi)\phi(\xi) - D \int_\Gamma \phi^* \frac{\partial \phi}{\partial n} d\Gamma + D \int_\Gamma \phi \frac{\partial \phi^*}{\partial n} d\Gamma + \int_\Gamma \phi \phi^* \bar{\upsilon}_n d\Gamma \tag{15}$$

$$= \sum_{k=1}^{M} \alpha_k \left[c(\xi)\psi_k(\xi) - D \int_\Gamma \phi^* \frac{\partial \psi_k}{\partial n} d\Gamma + D \int_\Gamma \psi_k \frac{\partial \phi^*}{\partial n} d\Gamma + \int_\Gamma \psi_k \phi^* \bar{\upsilon}_n d\Gamma \right]$$