



Dual reciprocity boundary element analysis of transient advection-diffusion

Dual reciprocity

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Abstract *This paper presents an application of the dual reciprocity boundary element method (DRBEM) to transient advection-diffusion problems. Radial basis functions and augmented thin plate splines (TPS) have been used as coordinate functions in DRBEM approximation in addition to the ones previously used in the literature. Linear multistep methods have been used for time integration of differential algebraic boundary element system. Numerical results are presented for the standard test problem of advection-diffusion of a sharp front. Use of TPS yields the most accurate results. Further, considerable damping is seen in the results with one step backward difference method, whereas higher order methods produce perceptible numerical dispersion for advection-dominated problems.*

1. Introduction

The phenomenon of advection-diffusion is observed in many physical situations involving transport of energy and chemical species. Some of the examples are the transport of pollutants – thermal, chemical or radioactive – in the environment, flow in porous media, impurity redistribution in semiconductors, travelling magnetic field etc. The governing equation for advection-diffusion is usually characterized by a dimensionless parameter, called Peclet number, Pe , which is defined as

$$Pe = |v| \frac{L}{D}, \quad (1)$$

where v is the advective velocity, L is the characteristic length and D is the diffusivity associated with the transport process. When Pe is small, diffusion



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dominates and the advection-diffusion equation is nearly parabolic. On the other hand, if Pe is large, then advection dominates and the governing equation becomes hyperbolic. Accurate numerical solution of the advection-diffusion equation becomes increasingly difficult as the Pe increases due to the onset of spurious oscillations or excessive numerical damping, if standard finite difference or finite element formulations are used. To deal with such advection dominated problems, numerous innovative algorithms have been suggested based on the local analytical solution of the advection-diffusion equation in the finite difference and finite element literature (Carey and Jiang, 1988; Celia *et al.*, 1989; Chen and Chen, 1984; Demkowicz and Oden, 1986; Ding and Liu, 1989; Donea *et al.*, 1984; Hughes and Brooks, 1982; Li *et al.*, 1992; Park and Liggett, 1990; Raithby and Torrance, 1974; Spalding, 1972; Westerink and Shea, 1989; Yu and Heinrich, 1986).

The reduction in the effective dimensionality of a problem offered by the boundary element method has attracted its application to the advection-diffusion problem as well, and it has been observed that the BEM solutions seem to be *relatively free* from spurious oscillations or excessive numerical damping (vis-à-vis finite element or finite difference solutions). The basic reason being the correct amount of upwinding provided by the fundamental solution in the BEM. Various formulations have been proposed for the transient advection-diffusion problems. Boundary element formulations based on time-dependent fundamental solutions have been suggested by Brebbia and Skerget (1984) and Ikeuchi and Onishi (1983). Ikeuchi and Onishi (1983) derived time-dependent fundamental solution to the advection-diffusion equation in \mathbf{R}^n , and proved that the boundary element solution is stable for large diffusion number and Courant number. This formulation is used by Ikeuchi and Tanaka (1985) for the solution of magnetic field problems. Tanaka *et al.* (1987) used the same formulation with mixed boundary elements and studied the dependence of the relative error on space and time discretization. On the other hand, Brebbia and Skerget (1984) used the fundamental solution of diffusion equation and treated the convective terms as a pseudo source term. Okamoto (1989, 1991) used Laplace transforms in conjunction with combined boundary and finite element methods for the solution of transient advection-diffusion problem on an unbounded domain.

Another class of boundary element formulations use the fundamental solution of a related steady-state operator and treat the time derivative and any other remaining terms as a pseudo source term. These formulations result in a system of differential-algebraic equations in time which can be solved using a suitable time integration algorithm. Taigbenu and Liggett (1986) proposed one such formulation. They use the fundamental solution of Laplace equation and treat the time derivative and convective terms as source terms which are incorporated in the boundary element formulation by domain discretization. Single step time-differencing scheme is used for time marching and solutions

are presented for a wide range of Pe – from very low (diffusion-dominated problems) to infinite (pure advection problems). Aral and Tang (1989) also used the fundamental solution of the Laplace equation, but made use of a secondary reduction process, called SR-BEM (Aral and Tang, 1988), to arrive at a boundary-only formulation. They present the results of the advection-diffusion problems with or without first order chemical reaction for low to moderate Pe . Two other formulations in this category are based on the dual reciprocity boundary element method (DRBEM) (Partridge *et al.*, 1991). The first one employs the fundamental solution to Laplace equation and applies the dual reciprocity treatment to time derivative and convective terms. The second one uses the fundamental solution to the steady-state advection-diffusion equation and transforms the domain integral arising from the time derivative term using a set of coordinate functions and particular solutions which satisfy the associated nonhomogeneous steady-state advection-diffusion equation (DeFigueiredo and Wrobel, 1990). In both these formulations, the resulting differential-algebraic equation is solved using one step θ -method. Partridge *et al.* (1991) used $\theta = 0.5$ in computations with first formulation and $\theta = 1.0$, with the second one, and observed that the accuracy of both the dual reciprocity formulations is very good for all problems considered, with no oscillations and only a minor damping of the wave front. They further indicate that the second formulation is more accurate than the first one. However, all the DRBEM applications have considered only the problems involving low values of Pe .

In this work, we concentrate on the application of the DRBEM based on the fundamental solution to the steady-state advection-diffusion equation to obtain a clear picture of its performance for advection-diffusion problems involving moderate to high Pe , since advection-dominated problems have received little attention in DRBEM literature. Further, only a simple set of radial basis functions has been previously used in this formulation. We consider two other sets of coordinate functions – complete radial basis functions and augmented thin plate splines (TPS), and analyse their performance in conjunction with higher order time integration algorithms for advection-dominated problems. We start with a brief review of the governing equations and the boundary element formulation, give the description of the coordinate functions and time integration schemes and present numerical results for a standard test problem of advection-diffusion of a sharp front.

2. Advection-diffusion equation

Let us consider a homogeneous isotropic region $\Omega \subset \mathbf{R}^2$ bounded by a piece-wise smooth boundary Γ . Let ϕ be the transported quantity, and $(0, T] \subset \mathbf{R}$ be the time interval of interest. Let x represent the spatial coordinate, and t the time. The transport of ϕ in the presence of a first order reaction is governed by the equation

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla + k - D\nabla^2\right)\phi(x, t) = 0 \quad \text{in } \Omega \times (0, T], \quad (2)$$

with the initial condition

$$\phi(x, 0) = \phi_0(x) \quad \text{on } \bar{\Omega}, \quad (3)$$

and the boundary conditions

$$\phi(x, t) = \bar{\phi}(x, t) \quad \text{on } \Gamma_\phi \times (0, T], \quad (4)$$

$$q(x, t) = \bar{q}(x, t) \quad \text{on } \Gamma_q \times (0, T], \quad (5)$$

$$q(x, t) = h(x, t)\{\phi_r(x, t) - \phi(x, t)\} \quad \text{on } \Gamma_r \times (0, T], \quad (6)$$

where v denotes the velocity field, D is the diffusivity and k is the reaction rate. ϕ_0 , $\bar{\phi}$, \bar{q} , ϕ_r and h are known functions and $q = \partial\phi/\partial n$, \mathbf{n} being the unit outward normal. Further, Γ_ϕ , Γ_q and Γ_r denote the disjoint segments (some of which may be empty) of the boundary such that $\bar{\Gamma}_\phi \cup \bar{\Gamma}_q \cup \bar{\Gamma}_r = \Gamma$. In this work, we assume that the advective velocity v and diffusivity D remain constant.

3. Boundary element formulation

This section presents a brief review of the dual reciprocity boundary element formulation for transient advection-diffusion based on the fundamental solution of the steady-state advection-diffusion equation. Further details are given in DeFigueiredo and Wrobel (1990) and Partridge *et al.* (1991).

To transform the advection-diffusion equation (2) into an equivalent boundary integral equation, we start with the weighted residual statement

$$\int_{\Omega} \left(\frac{\partial \phi}{\partial t} + v \cdot \nabla \phi + k\phi - D\nabla^2 \phi\right) \phi^* \, d\Omega = 0, \quad (7)$$

where ϕ^* is the fundamental solution of the steady-state advection-diffusion equation, i.e. the solution of

$$D\nabla^2 \phi^* + v \cdot \nabla \phi^* - k\phi^* + \delta(\xi, x) = 0. \quad (8)$$

In the preceding equation, δ is the Dirac delta function, and ξ and x denote the source and field points, respectively. For two-dimensional problems, ϕ^* is given by (Partridge *et al.*, 1991)

$$\phi^* = \frac{1}{2\pi D} \exp\left(-\frac{v \cdot r}{2D}\right) K_0(\mu r), \quad (9)$$

where

$$\mu = \left[\left(\frac{|v|}{2D} \right)^2 + \frac{k}{D} \right]^{1/2}, \quad (10)$$

and K_0 is the Bessel function of the second kind of order zero. Application of Green's second identity and relation (8) to the statement (7) yields

$$c_i \phi_i + D \int_{\Gamma} \left[\left(q^* + \frac{v_n}{D} \phi^* \right) \phi - \phi^* q \right] d\Gamma = - \int_{\Omega} \frac{\partial \phi}{\partial t} \phi^* d\Omega, \quad (11)$$

where the index i stands for the source point ξ , $q^* = \partial \phi^* / \partial n$, $v_n = v \cdot \mathbf{n}$ and

$$c_i = \int_{\Omega} \delta(\xi, x) d\Omega.$$

To transform the domain integral in equation (11), the time derivative is approximated by

$$\dot{\phi} = \sum_{j=1}^{NP} f^j(x) \alpha^j(t), \quad (12)$$

where the dot $\dot{\phi}$ on denotes the temporal derivative, α^j are unknown functions of time and f^j are known coordinate functions. Further, it is assumed that for each function f^j , there exists a function ψ^j which is a particular integral of the equation

$$D \nabla^2 \psi - v \cdot \nabla \psi - k \psi = f. \quad (13)$$

Introducing approximation (12) into equation (11) and applying integration by parts, we obtain the following boundary integral equation:

$$\begin{aligned} c_i \phi_i + D \int_{\Gamma} \left[\left(q^* + \frac{v_n}{D} \phi^* \right) \phi - \phi^* q \right] d\Gamma \\ = \sum_{j=1}^{NP} \alpha^j \left\{ c_i \psi_i^j + D \int_{\Gamma} \left[\left(q^* + \frac{v_n}{D} \phi^* \right) \psi^j - \phi^* \eta^j \right] d\Gamma \right\}, \quad (14) \end{aligned}$$

where $\eta^j = \partial \psi^j / \partial n$.

Application of the standard boundary element discretization procedure and approximation of ϕ , q , ψ , and η by the same set of interpolation functions within each boundary element followed by the collocation of the discretized boundary integral equation at all the freedom nodes (boundary plus internal) results in the system of equations

$$\mathbf{H}\boldsymbol{\phi} - \mathbf{G}\mathbf{q} = (\mathbf{H}\boldsymbol{\Psi} - \mathbf{G}\mathbf{E})\boldsymbol{\alpha}, \quad (15)$$

where \mathbf{H} and \mathbf{G} are the global matrices of the boundary integrals with kernels $(q^* + v_n \phi^*/D)$ and ϕ^* , respectively; $\mathbf{\Psi}$ and \mathbf{E} are the coordinate function matrices of functions ψ and η , respectively; and $\mathbf{\alpha}$, $\mathbf{\phi}$ and \mathbf{q} denote global nodal vectors of respective functions. Equation (12) can be used to eliminate $\mathbf{\alpha}$ from the preceding equation and thus, obtain the differential algebraic system

$$\mathbf{C}\mathbf{\phi} + \mathbf{H}\mathbf{\phi} - \mathbf{G}\mathbf{q} = 0, \tag{16}$$

where $\mathbf{C} = (\mathbf{G}\mathbf{E} - \mathbf{H}\mathbf{\Psi})\mathbf{F}^{-1}$, \mathbf{F} being the coordinate function matrix of the functions f^j .

4. Coordinate functions

Various sets of coordinate functions have been used in the dual reciprocity method for different class of problems. These include radial basis functions, TPS, multiquadrics etc. (Goldberg *et al.*, 1996, 1998). However, in the case of the dual reciprocity formulation for the advection-diffusion problems based on the fundamental solution of the steady-state advection-diffusion equation, the situation is quite different, probably due to the difficulty in obtaining closed form particular solutions to equation (13) for a given choice of f^j . Only the following set of coordinate functions has been used so far (DeFigueiredo and Wrobel, 1990):

$$\psi = r^3, \quad \eta = 3r \mathbf{r} \cdot \mathbf{n}, \quad f = 9Dr - 3r \mathbf{r} \cdot v - kr^3. \tag{17}$$

To obtain the preceding set, DeFigueiredo and Wrobel (1990) choose function ψ and obtained η and f by substituting directly into equation (13). This set would be referred to as RBF1 hereafter. This choice of the particular solution ψ essentially corresponds to the choice of $f = 9r$ for the Poisson's equation. We can follow the same approach to obtain the other sets of coordinate functions. We consider two more alternative sets corresponding to $f = 1 + r$ and augmented TPS for the Poisson's equation, both of which are known to possess better interpolation properties (Goldberg *et al.*, 1998), and thus are likely to yield more accurate results in the present context as well. If we choose $\psi = r^2/4 + r^3/9$, corresponding to the choice of $f = 1 + r$ for Poisson's equation, we can obtain the following set (which would be referred to as RBF2):

$$\begin{aligned} \psi &= r^2/4 + r^3/9, \\ \eta &= (1/2 + r/3)\mathbf{r} \cdot \mathbf{n}, \\ f &= D(1 + r) - (1/2 + r/3)\mathbf{r} \cdot v - k(9r^2 + 4r^3)/36. \end{aligned} \tag{18}$$

Further, if we choose ψ corresponding to augmented TPS for the Poisson's equation, we obtain the following set:

$$\psi = r^4(2 \log r - 1)/32 + r^2/4 + r^3/9,$$

$$\eta = (12r^2 \log r - 3r^2 + 16r + 24) \mathbf{r} \cdot \mathbf{n}/48, \quad (19)$$

$$f = D(1 + r + r^2 \log r) - (12r^2 \log r - 3r^2 + 16r + 24) \mathbf{r} \cdot \mathbf{v}/48 - k\psi.$$

5. Temporal discretization

The differential algebraic system (16) has a form similar to the one obtained using the finite element method and hence, can be solved by any standard time integration scheme by incorporating suitable modifications to account for its *mixed-nature*. Based on our previous experience (Singh and Kalra, 1996; Singh and Tanaka, 1998), we opt for one and multistep θ -methods of SS p 1 family (Wood, 1990) in this work. Further details on the temporal discretization aspects are available in Singh and Kalra (1996) and Singh and Tanaka (1998).

The general form of a p -step algorithm of SS p 1 family (Zienkiewicz *et al.*, 1984) for the differential-algebraic boundary element system (16) can be expressed as

$$\sum_{j=0}^p \{(\gamma_j \mathbf{C} + \beta_j \Delta t \mathbf{H}) \phi_{\alpha_j} - \beta_j \Delta t \mathbf{G} \mathbf{q}_{\alpha_j}\} = 0, \quad (20)$$

where $\alpha_j = n + j + 1 - p$, and γ_j, β_j are scalar coefficients which can be expressed as functions of p θ -parameters (Wood, 1990). Table I lists some schemes of this family and related parameters. The choice of the schemes has been made keeping in view the stringent stability requirements of a differential algebraic system. Of these algorithms, one step backward difference scheme is the most stable, but the least accurate. The Crank-Nicolson scheme is supposed to be the most accurate amongst the linear multistep methods, but is only marginally stable and prone to oscillations. Two and three step backward difference methods are likely to provide a compromise on accuracy and algorithmic damping.

Algorithm	Abbreviations	Parameters
Crank-Nicolson method	SS1C	$\theta = 1/2$
One step backward difference	SS1B	$\theta = 1$
Two step backward difference	SS2B	$\theta_1 = 1.5, \theta_2 = 2$
Three step backward difference	SS3B	$\theta_1 = 2, \theta_2 = 11/3, \theta_3 = 6$

Table I.
Time integration algorithms from SS p 1 family for advection-diffusion problem

Let us note that the multistep methods require additional starting values. Use of a higher order single step scheme such as the Runge-Kutta method is generally recommended in the literature for the generation of these additional initial conditions. However, numerical experiments by Singh and Kalra (1996) show that the higher order one step schemes are prone to numerical oscillations for differential-algebraic systems. Hence, we opt for the one step backward difference method with a reduced time step to generate additional starting values.

6. Error indicators

To measure the quality of the approximate solution, we need to utilize some appropriate norms. In the context of the boundary element analysis, the boundary L_2 norm is usually preferred, as it can be easily evaluated from the boundary solution alone in contrast to the energy norm which requires solutions to be known at internal points as well (Rencis and Jong, 1989).

The absolute error in the approximate solution of function v is defined as

$$e_v(x, t) = v(x, t) - v_a(x, t), \quad (21)$$

where $v(x, t)$ denotes the exact value and $v_a(x, t)$ is the approximate value obtained from the boundary element analysis. The L_2 global error norm is defined by

$$\|e_v\|_2^2 = \int_{\Gamma} e_v^2 d\Gamma = \sum_{i=1}^{N_e} \int_{\Gamma_i} e_v^2 d\Gamma, \quad (22)$$

where N_e is the total number of boundary elements. To obtain a more transparent measure of solution error, exact relative L_2 error (in per cent) can be defined as (Rencis and Jong, 1989)

$$\eta_v = \frac{\|e_v\|_2}{\|v\|_2} \times 100, \quad (23)$$

in which

$$\|v\|_2^2 = \int_{\Gamma} v^2 d\Gamma.$$

For the computation of L_2 -norms, we have used Gaussian quadrature with 24 integration points.

7. Numerical results

Let us consider the standard test problem of advection-diffusion of a sharp front along a line in uniform flow with the initial condition

$$\phi(x_1, 0) = 0 \quad x_1 \in [0, \infty), \quad (24) \quad \text{Dual reciprocity}$$

and the boundary conditions

$$\phi(0, t) = 1, \quad \phi(\infty, t) = 0. \quad (25)$$

With uniform advective velocity u , and absence of external or internal sources and reaction term, the exact solution of this problem is given by

$$\phi(x_1, t) = \frac{1}{2} \left[\operatorname{erfc}(z_1) + \exp\left(\frac{ux_1}{D}\right) \cdot \operatorname{erfc}(z_2) \right], \quad (26)$$

where $z_1 = (x_1 - ut)/\sqrt{4Dt}$ and $z_2 = (x_1 + ut)/\sqrt{4Dt}$. This problem is modelled as a two-dimensional problem over the rectangular domain Ω defined as

$$\Omega = \{(x_1, x_2) : x_1 \in (0, 1), x_2 \in (0, 0.1)\}, \quad (27)$$

with the zero initial condition. Boundary conditions are: $\phi(x, t) = 1$ on the boundary $x_1 = 0$; $q(x, t) = 0$ along upper ($x_2 = 0.1$) and lower boundary ($x_2 = 0$); and $\phi(x, t) = 0$ on the boundary $x_1 = 1$. The last boundary condition represents an approximation of the boundary condition $\phi(\infty, t) = 0$.

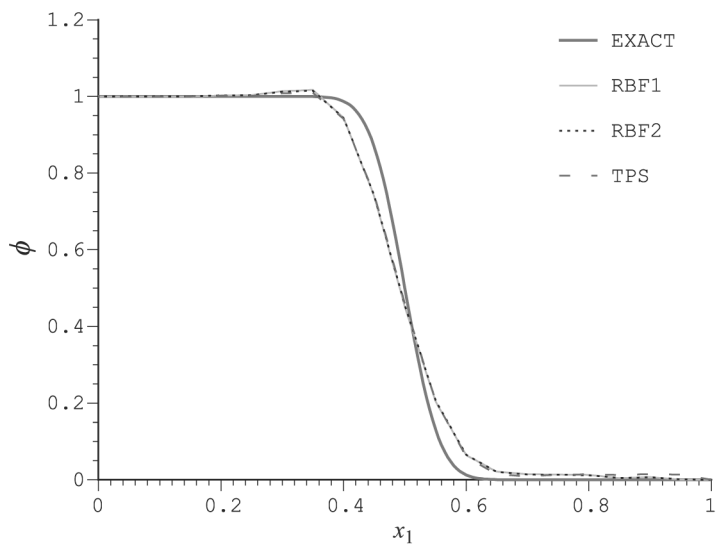
Equal linear elements ($\Delta\Gamma = 0.05$) have been used for the discretisation of the boundary Γ , with partially discontinuous elements at the corners. We take $u = 1.0$, and thus with the unit value of the characteristic length L , $Pe = 1/D$. We present results with two values of D which correspond to $Pe = 500$, and 1,000, respectively. These two cases represent moderate to heavily advection-dominated transport process.

We summarize the errors in the numerical solutions for both the cases for different sets of the coordinate functions in Table II. It can be observed that for both the problems, the higher order multistep methods produce very accurate results, and the three step backward difference scheme is the most accurate. Further, choice of augmented TPS as coordinate functions yields the most accurate results, whereas the previously used choice, RBF1, is the least accurate.

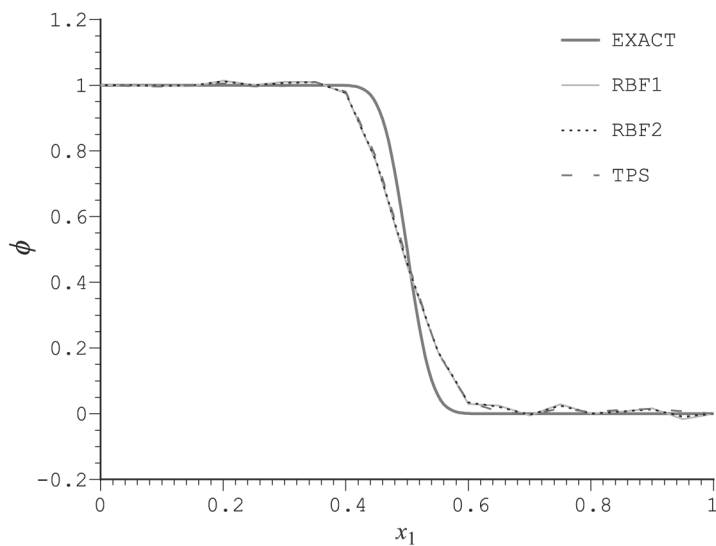
Figures 1 and 2 present the profile of the sharp front at $t = 0.5$ with SS1B and SS3B, respectively. For both the cases, considerable damping of the front is observed with the one step backward difference method, whereas perceptible

Scheme	Relative L_2 error (per cent) with $\Delta t = 0.005$					
	Pe = 500			Pe = 1,000		
	RBF1	RBF2	TPS	RBF1	RBF2	TPS
SS1B	6.11	6.07	5.96	8.15	8.06	7.72
SS1C	4.29	4.07	3.81	6.08	5.75	5.18
SS2B	3.88	3.68	3.41	5.81	5.50	4.97
SS3B	3.60	3.41	3.18	5.50	5.18	4.67

Table II.
Errors in the boundary element solution of sharp front problem for Pe = 500 and 1,000 ($t = 0.5$)



(a) $Pe = 500$



(b) $Pe = 1,000$

Figure 1.
Profile of the sharp front
at $t = 0.5$ with SS1B and
different coordinate
functions. (a) $Pe = 500$
and (b) $Pe = 1,000$
($\Delta t = 0.005$)

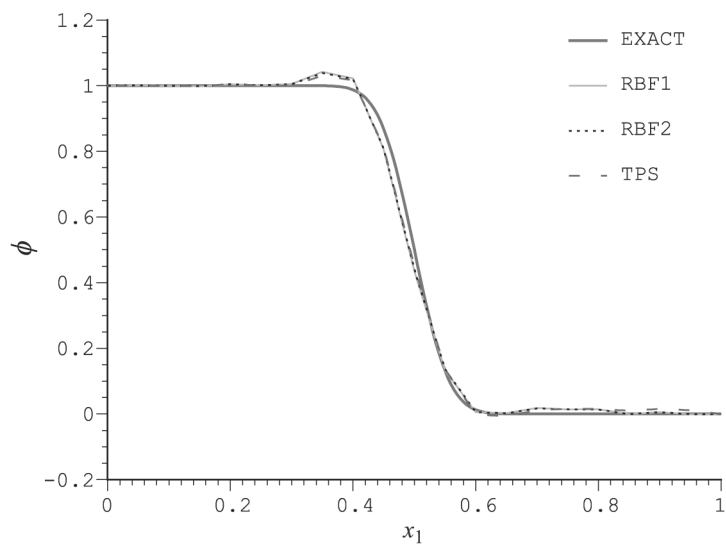
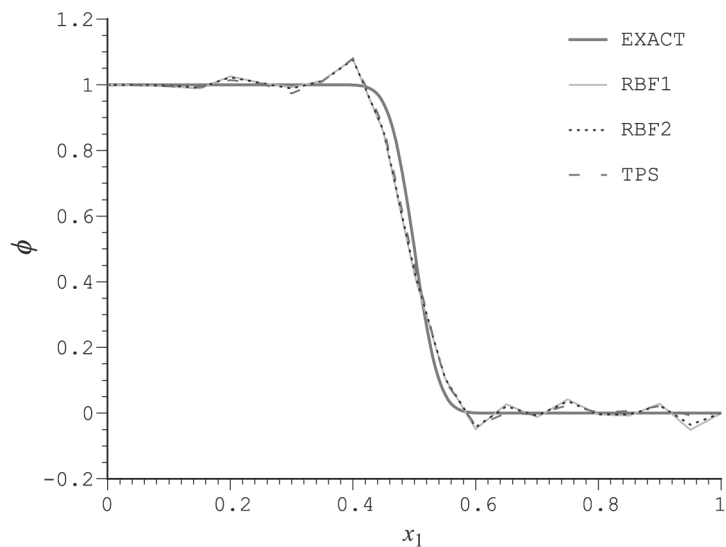
(a) $Pe = 500$ (b) $Pe = 1,000$

Figure 2. Profile of the sharp front at $t = 0.5$ with SS3B and different coordinate functions ($\Delta t = 0.005$)

numerical dispersion is present in the solution with SS3B (results with other two higher order schemes are very similar).

8. Concluding remarks

We have presented an application DRBEM to the transient advection-diffusion problems. In addition to the previously used set of coordinate functions of radial basis type, two more sets of coordinate functions – the radial basis and TPS type – have been evaluated. Of these, the use of the augmented TPS yields the most accurate results. Linear multistep methods have been used for time integration of the differential algebraic boundary element system. Of these, one step backward difference method produces considerable damping of the wave front. The higher order schemes yield good overall accuracy, although some numerical dispersion is present in the solution for the advection-dominated problems.

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