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An evaluation of boundary element schemes for convection-diffusion problems

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ABSTRACT

This paper presents a numerical evaluation of the performance of three different boundary element schemes for solving steady-state convection-diffusion problems with variable velocity fields. Two of these schemes are based on the dual reciprocity BEM: the first uses the fundamental solution of Laplace's equation and treats the whole convective part through the DRM; the other decomposes the velocity field into an average and a perturbation, and uses the fundamental solution of the convection-diffusion equation for constant velocity. In this case, only the perturbation is treated using a dual reciprocity approximation. The third scheme also decomposes the velocity field into an average and a perturbation, but the effects of the perturbation velocity are included through domain discretization. A comparison of the performance of the three schemes is presented for two different problems.

INTRODUCTION

A substantial number of numerical models for the convection-diffusion equation has appeared in the literature. Most of these models employ either the finite difference or the finite element methods of solution, and give emphasis on algorithms to suppress the well-known problems of oscillations and damping of wave fronts intrinsic to these methods [1].

Applications of the boundary element method for convection-diffusion have shown that the BEM is free from these problems [2-4]. This is due to the correct degree of "upwind" present in the fundamental solution of the convection-diffusion equation [5]. The main restriction of the BEM formulation, however, is the fact that fundamental solutions are only available for equations with constant coefficients, or coefficients with very simple variations in space [6].

Formulations for treating problems with variable velocity fields have employed the fundamental solution of Laplace's equation and treated the convective terms as pseudo-sources [7-9], or using the DRM [10]. Alternatively, the velocity field can be decomposed into an average and a perturbation, and the fundamental solution of the convection-diffusion equation employed incorporating the average velocity. The perturbation field can then be accounted for either by domain discretization [9,11] or through a DRM approximation [11].

In this paper, an evaluation is carried out on the numerical performance of three of the above schemes, as follows:

- Scheme 1, developed by Partridge and Brebbia [10], employs the fundamental solution of Laplace's equation and treats the whole convective terms through the DRM;
- Scheme 2, developed by Wrobel and DeFigueiredo [11], adopts the fundamental solution of the convection-diffusion equation incorporating the average velocity and treats the perturbation field using the DRM;
- Scheme 3, as scheme 2, uses the fundamental solution of the convection-diffusion equation with the average velocity but treats the perturbation field by domain discretization.

The next section presents a brief review of each method; this is followed by applications to two different problems, for which the performance of each scheme is compared and evaluated.

BOUNDARY ELEMENT FORMULATION

The two-dimensional steady-state convection-diffusion equation including first-order reaction can be written in the form

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

where $v_x = v_x(x,y)$ and $v_y = v_y(x,y)$ are the components of the velocity vector $\mathbf{v}$, D is the diffusivity coefficient (assuming the medium is homogeneous and isotropic) and k represents the reaction coefficient. 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. The mathematical description of the problem is complemented by boundary conditions of the Dirichlet, Neumann or Robin (mixed) types.

In order to obtain an integral equation equivalent to the above partial differential equation, a fundamental solution of equation (1) is necessary. However, fundamental solutions are only available for constant velocity fields.

One possibility is to use the fundamental solution of Laplace's equation and treat the convection and reaction terms as pseudo-sources, in the form

$$\nabla^2\phi = \frac{1}{D}\left(v_x\frac{\partial \phi}{\partial x} + v_y\frac{\partial \phi}{\partial y} + k\phi\right) \tag{2}$$

The equivalent boundary integral equation can be written as [10]:

$$c(\xi)\phi(\xi) - \int_\Gamma \phi^*\frac{\partial \phi}{\partial n}d\Gamma + \int_\Gamma \phi\frac{\partial \phi^*}{\partial n}d\Gamma = -\frac{1}{D}\int_\Omega \left(v_x\frac{\partial \phi}{\partial x} + v_y\frac{\partial \phi}{\partial y} + k\phi\right)\phi^* d\Omega \tag{3}$$

with ϕ^* the fundamental solution of Laplace's equation.

Alternatively, the variable velocity components $v_x(x,y)$ and $v_y(x,y)$ can be decomposed into average (constant) terms $\overline{v}_x$ and $\overline{v}_y$ and perturbations $P_x = P_x(x,y)$ and $P_y = P_y(x,y)$, *i.e.*

$$\begin{aligned} v_x(x,y) &= \overline{v}_x + P_x(x,y) \\ v_y(x,y) &= \overline{v}_y + P_y(x,y) \end{aligned}$$

This permits rewriting equation (1) as

$$D\nabla^2\phi - \overline{v}_x \frac{\partial\phi}{\partial x} - \overline{v}_y \frac{\partial\phi}{\partial y} - k\phi = P_x \frac{\partial\phi}{\partial x} + P_y \frac{\partial\phi}{\partial y} \qquad (4)$$

The above differential equation can now be transformed into the following boundary integral equation [11]:

$$c(\xi)\phi(\xi) - D\int_\Gamma \phi^* \frac{\partial\phi}{\partial n} d\Gamma + D\int_\Gamma \phi \frac{\partial\phi^*}{\partial n} d\Gamma + \int_\Gamma \phi\phi^* \overline{v}_n d\Gamma = - \int_\Omega \left(P_x \frac{\partial\phi}{\partial x} + P_y \frac{\partial\phi}{\partial y} \right) \phi^* d\Omega \qquad (5)$$

where $\overline{v}_n = \overline{\mathbf{v}}\cdot\mathbf{n}$, $\mathbf{n}$ is the unit outward normal vector and the dot stands for scalar product.

In the above equation, ϕ^* is now the fundamental solution of the convection-diffusion equation with constant coefficients, given by

$$\phi^*(\xi,\chi) = \frac{1}{2\pi D} e^{-\frac{\overline{\mathbf{v}}\cdot\mathbf{r}}{2D}} K_0(\mu r)$$

where

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

and r is the modulus of $\mathbf{r}$, the distance vector between the source and field points. Function K_0 is the Bessel function of second kind of order zero. The exponential term is responsible for inclusion of the correct amount of 'upwind' into the formulation [5].

DUAL RECIPROCITY APPROACHES

In order to obtain a boundary integral which is equivalent to the domain integral in equations (3) and (5), a dual reciprocity approximation can be introduced [12]. Considering initially the non-homogeneous term on the right-hand side of equation (5), the first step is its expansion into the following series,

$$P_x \frac{\partial\phi}{\partial x} + P_y \frac{\partial\phi}{\partial y} = \sum_{k=1}^{M} f_k\, \alpha_k \qquad (6)$$

The above series involves a sequence of known functions $f_k = f_k(x,y)$ which are dependent only on geometry, and a set of unknown coefficients α_k. With this approximation, the domain integral in equation (5) becomes

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$$\int_\Omega \left(P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y}\right) \phi^* d\Omega = \sum_{k=1}^{M} \alpha_k \int_\Omega f_k \phi^* d\Omega \tag{7}$$

It is then considered that, for each function f_k, there exists a related function ψ_k which is a particular solution of the equation

$$D\nabla^2\psi - \overline{v}_x \frac{\partial \psi}{\partial x} - \overline{v}_y \frac{\partial \psi}{\partial y} - k\psi = f \tag{8}$$

Thus, the domain integral can be recast in the form

$$\int_\Omega \left(P_x \frac{\partial \phi}{\partial x} + P_y \frac{\partial \phi}{\partial y}\right) \phi^* d\Omega =$$

$$\sum_{k=1}^{M} \alpha_k \int_\Omega \left(D\nabla^2\psi_k - \overline{v}_x \frac{\partial \psi_k}{\partial x} - \overline{v}_y \frac{\partial \psi_k}{\partial y} - k\psi_k\right) \phi^* d\Omega \tag{9}$$

Substituting expansion (9) into equation (5), and applying integration by parts to the domain integral of the resulting equation, one finally arrives at a boundary integral equation of the form

$$c(\xi)\phi(\xi) - D\int_\Gamma \phi^* \frac{\partial \phi}{\partial n} d\Gamma + D\int_\Gamma \phi \frac{\partial \phi^*}{\partial n} d\Gamma + \int_\Gamma \phi\phi^* \overline{v}_n d\Gamma =$$

$$\sum_{k=1}^{M} \alpha_k \left[c(\xi)\psi_k(\xi) - D\int_\Gamma \phi^* \frac{\partial \psi_k}{\partial n} d\Gamma + D\int_\Gamma \psi_k \frac{\partial \phi^*}{\partial n} d\Gamma + \int_\Gamma \psi_k \phi^* \overline{v}_n d\Gamma\right] \tag{10}$$

Applying the discretized version of equation (10) to all boundary nodes using a collocation technique results in the following system of equations:

$$\mathbf{H}\boldsymbol{\phi} - \mathbf{G}\mathbf{q} = (\mathbf{H}\boldsymbol{\psi} - \mathbf{G}\boldsymbol{\eta})\boldsymbol{\alpha} \tag{11}$$

with $q = \partial\phi/\partial n$ and $\eta = \partial\psi/\partial n$. In the above system, the same matrices $\mathbf{H}$ and $\mathbf{G}$ are used on both sides. Matrices $\boldsymbol{\psi}$ and $\boldsymbol{\eta}$ are geometry-dependent square matrices, while $\boldsymbol{\phi}$, $\mathbf{q}$ and $\boldsymbol{\alpha}$ are vectors of nodal values.

The next step in the formulation is to find an expression for the unknown vector $\boldsymbol{\alpha}$. Applying equation (6) to all M nodes, it is possible to write the resulting set of equations in the following matricial form,

$$\mathbf{P}_x \frac{\partial \boldsymbol{\phi}}{\partial x} + \mathbf{P}_y \frac{\partial \boldsymbol{\phi}}{\partial y} = \mathbf{F}\,\boldsymbol{\alpha} \tag{12}$$

where $\mathbf{P}_x$ and $\mathbf{P}_y$ are two diagonal matrices with components $P_x(x_i, y_i)$ and $P_y(x_i, y_i)$, $i = 1, ..., M$, while $\frac{\partial \boldsymbol{\phi}}{\partial x}$ and $\frac{\partial \boldsymbol{\phi}}{\partial y}$ are column vectors.

Writing expression (12) in terms of $\boldsymbol{\alpha}$ and substituting into equation (11) gives

$$\mathbf{H}\boldsymbol{\phi} - \mathbf{G}\mathbf{q} = \mathbf{S}\left(\mathbf{P}_x \frac{\partial \boldsymbol{\phi}}{\partial x} + \mathbf{P}_y \frac{\partial \boldsymbol{\phi}}{\partial y}\right) \tag{13}$$

with

$$\mathbf{S} = (\mathbf{H}\boldsymbol{\psi} - \mathbf{G}\boldsymbol{\eta})\,\mathbf{F}^{-1}$$

It can be noted that matrix $\mathbf{S}$ depends on geometry only, once the sequence of functions f_k has been defined. The coefficients of matrices $\mathbf{P}_x$ and $\mathbf{P}_y$ are also known. Thus, there remains to be found an expression relating the derivatives of $\boldsymbol{\phi}$ with nodal values of $\boldsymbol{\phi}$ to reduce equation (13) to a standard BEM form. Herein, the algorithm suggested by Partridge and Brebbia [10] is adopted.

By expanding the value of ϕ at an internal point using a similar approximation to expression (6), one obtains

$$\phi = \sum_{k=1}^{M} f_k \beta_k \tag{14}$$

Differentiating the above with respect to x and y produces

$$\frac{\partial \phi}{\partial x} = \sum_{k=1}^{M} \frac{\partial f_k}{\partial x} \beta_k \tag{15}$$

$$\frac{\partial \phi}{\partial y} = \sum_{k=1}^{M} \frac{\partial f_k}{\partial y} \beta_k \tag{16}$$

Applying equation (14) at all M nodes, inverting the resulting matrix and substituting the expression for $\boldsymbol{\beta}$ into the matrix forms of equations (15) and (16) gives

$$\frac{\partial \boldsymbol{\phi}}{\partial x} = \frac{\partial \mathbf{F}}{\partial \mathbf{x}} \mathbf{F}^{-1} \boldsymbol{\phi} \tag{17}$$

$$\frac{\partial \boldsymbol{\phi}}{\partial y} = \frac{\partial \mathbf{F}}{\partial \mathbf{y}} \mathbf{F}^{-1} \boldsymbol{\phi} \tag{18}$$

and equation (13) takes the form

$$(\mathbf{H} - \mathbf{P})\boldsymbol{\phi} = \mathbf{G}\mathbf{q} \tag{19}$$

where

$$\mathbf{P} = \mathbf{S}\left(\mathbf{P}_x \frac{\partial \mathbf{F}}{\partial \mathbf{x}} + \mathbf{P}_y \frac{\partial \mathbf{F}}{\partial \mathbf{y}}\right) \mathbf{F}^{-1}$$

The coefficients of the perturbation matrix $\mathbf{P}$ are all known. Thus, once boundary conditions are applied to equation (19), the resulting system of algebraic equations can be solved in standard form.

The DRM scheme for solution of equation (3) is very similar to the above. The final system of equations has the form

$$(\mathbf{H} - \mathbf{P} - \mathbf{R})\boldsymbol{\phi} = \mathbf{G}\mathbf{q} \tag{20}$$

where

$$\mathbf{P} = \mathbf{S}\left(\mathbf{V}_x \frac{\partial \mathbf{F}}{\partial \mathbf{x}} + \mathbf{V}_y \frac{\partial \mathbf{F}}{\partial \mathbf{y}}\right) \mathbf{F}^{-1}$$

and

$$\mathbf{R} = \mathbf{S}\mathbf{K}$$

in which $\mathbf{V}_x, \mathbf{V}_y$ and $\mathbf{K}$ are diagonal matrices containing the values of $v_x/D, v_y/D$ and k/D, respectively.

It is important to notice that, although the DRM approximations to equations (3) and (5) are formally similar, matrices $\mathbf{H}, \mathbf{G}, \mathbf{F}, \psi$ and η are not the same in both cases. Matrices $\mathbf{H}$ and $\mathbf{G}$ depend on the fundamental solution which is different for equations (3) and (5), while matrices $\mathbf{F}, \psi$ and η depend on the choice of approximating function f (which is also different, see [10] and [11]) and its relation to ψ (which is given by expression (8) for the case of equation (5), and by $\nabla^2\psi = f$ for equation (3)).

DOMAIN DISCRETIZATION APPROACH

The domain integral in equations (3) and (5) can also be directly evaluated by dividing the domain into cells. In this work, this is only considered for equation (5) since it has been shown in [9] that the Laplace fundamental solution presents oscillations when implemented in a domain discretization approach. Although it is possible, and in many cases more convenient, to integrate by parts the domain integral in (5) to work with internal values of ϕ rather than its derivatives [9,11], this introduces derivatives of P_x and P_y into the formulation. For incompressible fluids this new term, which appears in the form

$$\int_\Omega \left(\frac{\partial P_x}{\partial x} + \frac{\partial P_y}{\partial y}\right) \phi^* \phi d\Omega,$$

is zero because of mass continuity. However, to keep the formulation general as the velocity field in our first test problem does not satisfy mass continuity, the domain discretization formulation was implemented directly using equation (5).

For convenience of the numerical scheme the term between brackets on the domain integral of equation (5), $P_x\partial\phi/\partial x + P_y\partial\phi/\partial y$, is denoted b. This whole term is then approximated within each internal cell by using interpolation functions and nodal values. Applying the discretized form of equation (5) to all boundary nodes then produces the system of equations

$$\mathbf{H}\phi - \mathbf{G}\mathbf{q} = \mathbf{E}\mathbf{b} \tag{21}$$

relating boundary values of ϕ and q and internal values of b. This system has to be complemented by equations for evaluating b. These equations are of the form

$$b(\xi) = D\int_\Gamma \left(P_x\frac{\partial \phi^*}{\partial x} + P_y\frac{\partial \phi^*}{\partial y}\right)\frac{\partial \phi}{\partial n} d\Gamma - D\int_\Gamma \left(P_x\frac{\partial}{\partial x}\frac{\partial \phi^*}{\partial n} + P_y\frac{\partial}{\partial y}\frac{\partial \phi^*}{\partial n}\right)\phi d\Gamma -$$
$$\int_\Gamma \left(P_x\frac{\partial \phi^*}{\partial x} + P_y\frac{\partial \phi^*}{\partial y}\right)\phi \bar{v}_n d\Gamma - \int_\Omega \left(P_x\frac{\partial \phi^*}{\partial x} + P_y\frac{\partial \phi^*}{\partial y}\right) b d\Omega \tag{22}$$

The discretized form of this equation, once applied to all internal points, produces the system

$$\overline{\mathbf{H}}\phi - \overline{\mathbf{G}}\mathbf{q} = \overline{\mathbf{E}}\mathbf{b} \tag{23}$$

Because b is not a variable of physical interest, it can be eliminated from (21) and (23) to produce the final system

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$$(\mathbf{H} - \mathbf{E}\overline{\mathbf{E}}^{-1}\overline{\mathbf{H}})\phi = (\mathbf{G} - \mathbf{E}\overline{\mathbf{E}}^{-1}\overline{\mathbf{G}})\mathbf{q} \tag{24}$$

relating only boundary values.

APPLICATIONS

The formulations presented here were applied to the following two cases:

- A one-dimensional problem with uni-directional velocity field depending on the $x-$coordinate;
- A two-dimensional problem with uni-directional velocity field depending on the $y-$coordinate.

In both cases, the diffusivity coefficient D was assumed equal to one, for simplicity. The DRM code with Laplace's fundamental solution uses quadratic boundary elements while the others use linear elements.

One-dimensional problem

In this example the velocity v_x is a linear function of x expressed as

$$v_x(x) = k\,x + C_1$$

and the v_y component is equal to zero. The governing equation of the problem then takes the form

$$\nabla^2\phi - (k\,x + C_1)\frac{\partial \phi}{\partial x} - k\,\phi = 0 \tag{25}$$

A particular solution of equation (25) is given by

$$\phi = \overline{\phi}\, e^{\frac{k}{2}x^2 + C_1 x} \tag{26}$$

Imposing the boundary conditions $\phi = \phi_a$ at $x = 0$ and $\phi = \phi_b$ at $x = 1$, the constants $\overline{\phi}$ and C_1 in (26) can be evaluated as

$$\overline{\phi} = \phi_a \quad ; \quad C_1 = \ln\left(\frac{\phi_b}{\phi_a}\right) - \frac{k}{2}$$

and the velocity field becomes:

$$v_x = \ln\left(\frac{\phi_b}{\phi_a}\right) + k\left(x - \frac{1}{2}\right)$$

The problem region is modelled as a rectangle with dimensions 1×0.7. The quadratic elements discretization used 20 elements, 9 along each horizontal face and 1 along each vertical face. In case of linear elements, 38 were used with 17 on each horizontal face and 2 on each vertical face. The boundary conditions specify the values $\phi_a = 300$ and $\phi_b = 10$ along the faces $x = 0$ and $x = 1$, respectively, with no flux in the $y-$direction.

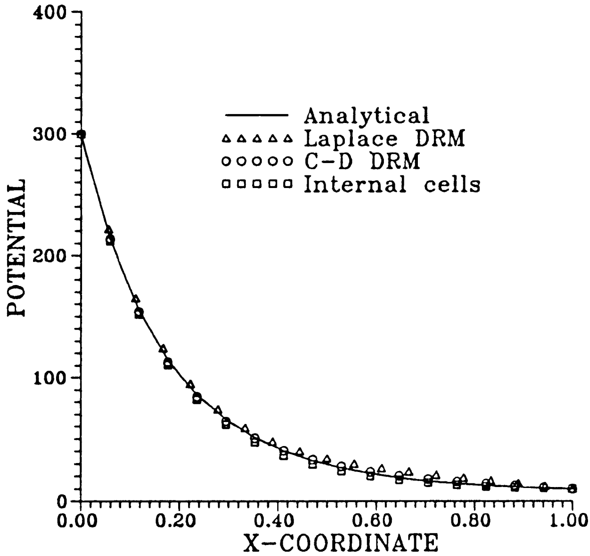

Figure 1: Potential distribution for $k = 5$

A plot of the variation of the potential ϕ along the $x-$axis is presented in figure 1 for $k = 5$. In this case, the velocity field is equal to $v_x = -3.401 \pm 2.5$. The DRM formulations did not use any internal point in the approximating series, while the cell formulation employed 8 linear rectangular cells. It can be seen that the agreement with the analytical solution is very good, with the Laplace fundamental solution producing slightly less accurate results.

Figures 2 and 3 present the cases $k = 20$ ($v_x = -3.401 \pm 10$) and $k = 40$ ($v_x = -3.401 \pm 20$). It is obvious that, as the velocity increases, the potential distribution becomes steeper and more difficult to reproduce with numerical models; thus, more refined discretizations are required. The DRM approximations employed 30 internal points for $k = 20$ and 54 for $k = 40$ while the cell formulation used 28 cells for both values of k. All solutions are still in good agreement for $k = 20$ but oscillations appear in both DRM formulations for $k = 40$, being more pronounced with the C-D fundamental solution than Laplace's. Results with the cell formulation are very good and display no oscillations whatsoever. It is important to remark that the cell formulation is convergent as the number of cells is increased, while both DRM formulations did not display monotonic convergence with increased numbers of internal points.

Two-dimensional problem

This example considers a uni-directional velocity field in the $x-$direction depending on y according to the expression

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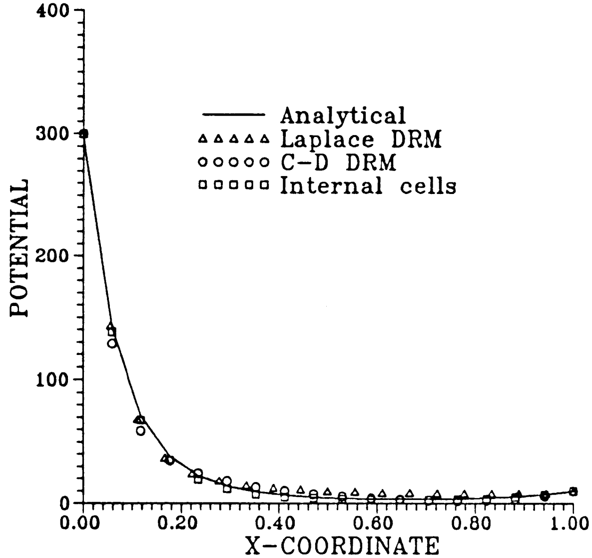

Figure 2: Potential distribution for $k = 20$

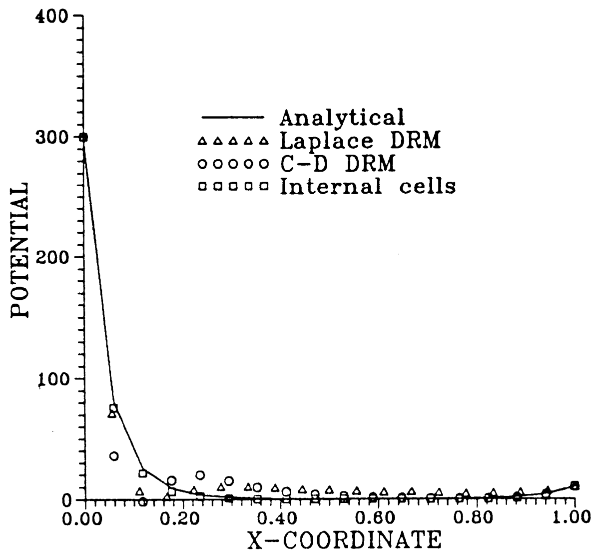

Figure 3: Potential distribution for $k = 40$

$$v_x(y) = \frac{\lambda^2}{C_2}(y-B)^2$$

with $\lambda = k - C_2^2$. The v_y component is again equal to zero and consequently the equation to be solved reduces to

$$\nabla^2\phi - \frac{\lambda^2}{C_2}(y-B)^2\frac{\partial\phi}{\partial x} - k\,\phi = 0 \tag{27}$$

A particular solution to the above equation is

$$\phi = \overline{\phi}\, e^{\frac{\lambda}{2}y^2 - \lambda By + C_2 x} \tag{28}$$

The value of the constant B defines the symmetry of the velocity field with respect to the coordinate y. If $B = 0.5$ the velocity and potential profiles are both symmetric.

The value of the constant C_2 is arbitrarily assumed as

$$C_2 = \ln\frac{\phi(1,0)}{\phi(0,0)}$$

with $\phi(0,0) = 300$ and $\phi(1,0) = 10$; the constant B is assumed equal to 0.5. This gives a symmetric, parabolic velocity field, with minimum at $y = 0.5$ ($v_x = 0$) and maximum at the extremes, the value of which is dependent on k.

The problem geometry is defined as a unit square with mixed boundary conditions prescribed according to expression (28), with the potential ϕ assumed known along the faces $x = 0$ and $x = 1$ and the flux $\partial\phi/\partial n$ given along the faces $y = 0$ and $y = 1$.

Figure 4 shows results for the potential ϕ along the faces $y = 0$ or $y = 1$ for the case of $k = 10$ (maximum velocity: $v_x = -0.181$). The boundary discretizations employed 20 quadratic or 40 linear elements, 5 or 10 along each face, with 18 internal points for the DRM formulations and 10 cells. It can be seen that all results are in excellent agreement.

Figures 5 and 6 show the cases of $k = 30$ (maximum velocity: $v_x = -24.98$) and $k = 50$ (maximum velocity: $v_x = -108.57$). Although the potential variation along $y = 0$ and $y = 1$ does not depend on k (expression (28) for $B = 0$), the internal variations are much steeper in these cases. Both DRM schemes produce reasonable results for $k = 30$, with the Laplace fundamental solution again displaying slightly larger errors; for $k = 50$, however, the C-D algorithm shows large oscillations while the Laplace fundamental solution does not, although the errors increase. The cell formulation is in excellent agreement with the analytical solution in all cases.

CONCLUSIONS

This paper has presented an assessment of three alternative BEM schemes for solution of convection-diffusion problems with variable velocity fields. The two DRM algorithms produce satisfactory results when the velocity field is low (*i.e.*

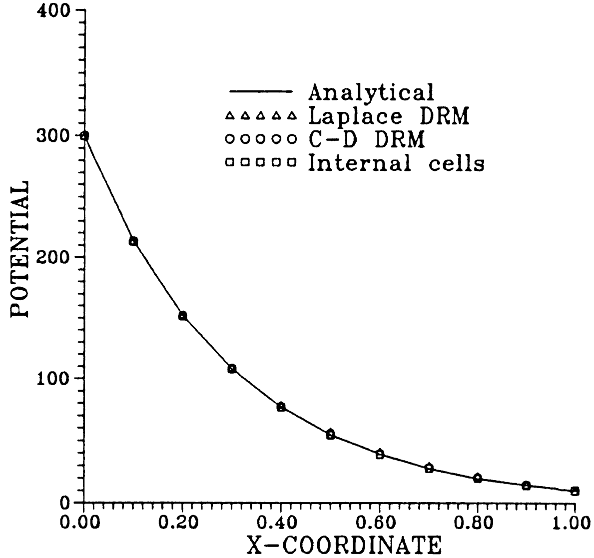

Figure 4: Potential distribution for $k = 10$

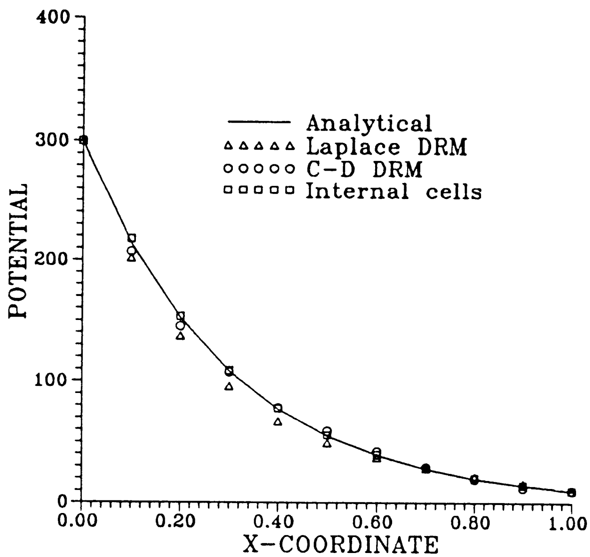

Figure 5: Potential distribution for $k = 30$

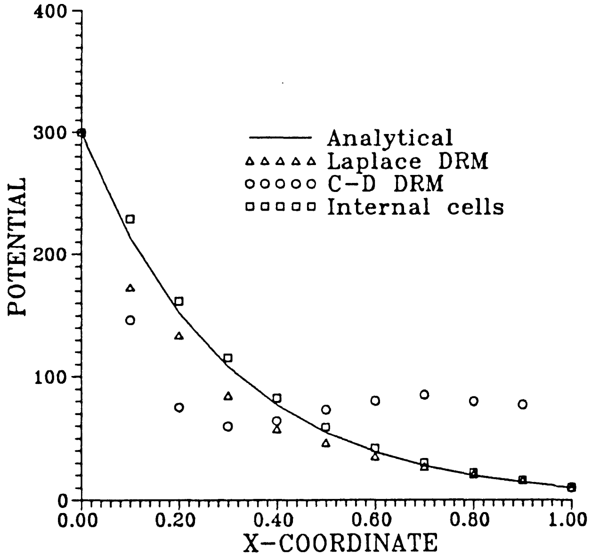

Figure 6: Potential distribution for $k = 50$

for diffusion-dominated problems) but may develop oscillations when velocities are high. Based on our experience, it appears that the main problem arises in the approximation of the partial derivatives of ϕ rather than ϕ itself; thus, alternative DRM formulations are being developed to avoid the need to approximate partial derivatives.

The cell formulation, on the other hand, presented very good results even for high velocity fields. The formulation, when implemented with the fundamental solution of the convection-diffusion equation with constant velocity, is convergent and does not produce oscillations. The solution of problems involving more complex velocity fields, including recirculation zones, will now be attempted with this formulation.

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