CHAPTER 1

Diffusion–convection problems

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Abstract

This chapter presents some solutions to the diffusion–convection equation that are based on the boundary element theory. Four formulations are discussed, but solutions from only three of them are presented. The formulations represent different replications of the differential equation along the lines of the singular integral theory. Their fundamental solutions come from different linear parts of the differential operator. The elliptic diffusion (ED) formulation that is based on the ED operator shows the most promise. Attempts at avoiding domain integrations through the dual reciprocity method are discussed, while full domain discretization through the Green element method for ease of evaluation of domain integrations and in solving heterogeneous and nonlinear transport is presented. The solutions from the three formulations to the nonlinear Burgers’ equation are also presented, with the ED formulation exhibiting superior performance.

1 Introduction

There are many transport phenomena of theoretical and practical interest in a number of fields of science and engineering that are governed by the diffusion–convection equation. It can, under certain conditions, describe transport of mass, momentum, vorticity, and energy when mechanisms of diffusion or dispersion and convection or advection are of importance. Its solution continues to attract considerable interest in numerical circles because of its unique feature of being either a parabolic or a hyperbolic equation, depending on the values of the parameters of
the equation, and also because its solution process offers valuable computational experience which can be extended to the simulation of many other flows of engineering interest.

Although there exist analytic solutions in one and two dimensions, their usefulness is limited to problems with simple regular geometries [1, 2]. Standard finite difference schemes produce, for advection-dominant cases, unacceptably large spurious oscillations or numerically diffused solutions [3–5]. From the reviews of finite element solutions provided by Anderson [6] and Zienkiewicz and Taylor [7], schemes that are based on Bobnov–Galerkin weighting functions showed similar spurious oscillations and diffused or smeared fronts because of their failure to correctly approximate the convective term. However, with upwind differencing of the convective term in what is now known as the Petrov–Galerkin weighting functions, more acceptable results have been reported [7–12].

Contemporary developments have been taking place in boundary element circles on accurate modeling of the transport equation. An earlier attempt by Brebbia and Skerget [13], which employed the fundamental solution to the temporal diffusion operator in two spatial dimensions, addressed only cases with small values of the Peclet number. Another approach, based on the fundamental solution to the 2D elliptic diffusion (ED) operator, treated the transient problem as a quasi-steady one and offered solutions which covered a wide spectrum of Peclet values [14–16]. All these formulations implemented the integral equations in the classical manner resulting in a fully populated global coefficient matrix.

It has been recognized that the boundary-only character of the boundary element theory, observed for elliptic problems and considered one of the strengths of the boundary element method (BEM), is not retained when dealing with a parabolic–hyperbolic equation like that of diffusion–convection. The dual reciprocity method (DRM), proposed by Nardini and Brebbia [17], provided a way of transforming the domain integrations into boundary ones, though the method requires that some nodal points within the domain be provided. The DRM was extended to diffusion–convection problems by Wrobel et al. [18] and Aral and Tang [19]. A number of domain discretization formulations are available, ranging from those that subdivide the computational region into subdomains that result in block-banded coefficient matrices [20] to those which subdivide the domain into elements, thereby achieving a banded coefficient matrix in a manner similar to that encountered in finite element methodology (FEM). The latter formulation is referred to as the Green element method (GEM) [21, 22]. These formulations are discussed in this chapter with reference to diffusion–convection problems.

A nonlinear form of the diffusion–convection equation is the Burgers’ equation. It provides a useful model for many diverse and seemingly unrelated phenomena such as shock flows, turbulence, wave propagation in combustion chambers, vehicular traffic movement, acoustic transmission, and many others. Boundary element formulations that have been applied to the Burgers’ equation are also discussed in this chapter.
2 Boundary element formulations

The mathematical statement of diffusion–convection transport in an incompressible medium can be written in general form as

\[ \nabla \cdot (D \nabla c) = \mathbf{u} \cdot \nabla c + \frac{\partial c}{\partial t} + Q \]  

(1)

where \( \nabla \) is the gradient operator, \( c \) is the basic dependent variable, \( D \) is a parameter that could depend on the medium (heterogeneous transport) and/or on the dependent variable (nonlinear transport), \( \mathbf{u} \) is the velocity vector, \( t \) is the time dimension, and \( Q \) represents the source term which could have a functional dependence on \( c \) as in reactive transport. It should be noted that the basic dependent variable need not be a scalar but could be a vector as in the case of transport of momentum. In the spatial dimension, eqn (1) could apply either to one or two or three dimensions. The uniqueness of the solutions to eqn (1) depends on the prescribed boundary and initial conditions. The first type or the Dirichlet boundary condition specifies the value of the dependent variable on a part of the boundary, i.e.

\[ c(\mathbf{r}, t) = C_1(t) \quad \text{on } \Gamma_1 \text{ for } t > t_0 \]  

(2a)

while the second type of boundary condition specifies the normal flux on another part

\[ D \nabla c \cdot \mathbf{n} = q_n(t) \quad \text{on } \Gamma_2 \text{ for } t > t_0 \]  

(2b)

where \( \mathbf{n} \) is the unit outward pointing normal vector on the boundary \( \Gamma = \Gamma_1 + \Gamma_2 \). The initial condition provides information on the distribution of \( c \) everywhere in the domain \( \Omega \), i.e.

\[ c(\mathbf{r}, t_0) = C_0(t) \quad \text{on } \Omega \]  

(2c)

Various boundary element solution strategies arise from the choice of Green’s function or the fundamental solution that is applied. All the approaches restate eqn (1) as

\[ L(c) = b \]  

(3)

where \( L \) stands for a linear differential part of eqn (1) and \( b \) can be referred to as a pseudo-forcing or source term that accounts for all heterogeneity and nonlinearity of the transport process. The solution to eqn (3) in an infinitely extensive spatial region is the free-space Green’s function or fundamental solution that is utilized in obtaining the integral representation of the transport equation. Different forms of eqn (3) have been used in boundary element methodology, and our discussion shall first be centered on the nontransient forms of \( L \).

2.1 Formulation with the ED operator

This formulation uses the nontransient portion of eqn (1) so that it can be rewritten as

\[ D \nabla^2 c = b \]  

(4)
where \( \overline{D} \) is some averaged value of the parameter \( D \) and the pseudo-force term \( b \) accounts for the convection, transient, and source terms.

\[
b = \mathbf{u} \cdot \nabla c + \frac{\partial c}{\partial t} + Q
\]  

(5)

The corresponding integral equation arising from applying Green’s identity to eqn (4) is

\[
\mathcal{D} \left( \lambda(\xi)c(\xi) + \int_{\Gamma} \left[ cG^* - G \frac{\partial c}{\partial n} \right] ds \right) + \iint_{\Omega} bGdA = 0
\]  

(6)

The function \( G \) refers to the fundamental solution or the solution of the linear operator

\[
\nabla^2 G + \delta(p, \xi) = 0
\]  

(7)

where \( \delta \) is the Dirac delta function, and \( G^* = \frac{\partial G}{\partial n} \) is the normal derivative of the fundamental solution. For the 2D case,

\[
G = -\frac{1}{2\pi} \ln r
\]  

(8a)

\[
G^* = -\frac{\eta}{2\pi r^2}
\]  

(8b)

and for the 3D case, it is

\[
G = \frac{1}{4\pi r}
\]  

(9a)

\[
G^* = -\frac{\eta}{4\pi r^3}
\]  

(9b)

where \( r = |\mathbf{r}| \) is the magnitude of the distance vector \( \mathbf{r} \) from the source point \( \xi \) to the field point \( p \), and \( \eta = \mathbf{r} \cdot \mathbf{n} \) is the normal distance from the source point to the boundary on which the field point is located. The parameter \( \lambda \) in eqn (6) has a value of unity if the source point is within the domain \( \Omega \), and, when the source point is on the boundary, it is a fractional value that depends on the nodal angle at the source point. The approach that is based on the ED operator has been applied by Taigbenu and Liggett [16], Aral and Tang [19], Popov and Power [23], among others. The solutions from the computer model based on the elliptic diffusion operator are referred to as ED in this chapter.

### 2.2 Formulation with the elliptic diffusion–convection (EDC) operator

This formulation is based on the nontransient ED and convection parts of eqn (1), i.e.

\[
\mathcal{D}\nabla^2 c - \mathbf{U} \cdot \nabla c = b
\]  

(10)

where \( \mathbf{U} \) is some reference uniform velocity field. In other words, the velocity vector \( \mathbf{u} \) has been decomposed into a uniform velocity vector \( \mathbf{U} \) and a perturbed one \( \hat{\mathbf{u}} \),
i.e. \( \mathbf{u} = \mathbf{U} + \mathbf{\hat{u}} \). The pseudo-force term \( b \) accounts for the perturbed convective velocity, transient, and source terms.

\[
 b = \mathbf{\hat{u}} \cdot \nabla c + \frac{\partial c}{\partial t} + Q 
\]

(11)

The corresponding integral equation for this formulation is similar to eqn (6) and it is given as

\[
\lambda(\zeta)c(\zeta) + \overline{D} \left( \int_{\Gamma} \left[ cG^* - \frac{\partial c}{\partial n} \right] ds \right) + \int_{\Gamma} c G U_n ds + \int \int_{\Omega} b G dA 
\]

(12)

where \( U_n = \mathbf{U} \cdot \mathbf{n} \) is the normal component of the uniform velocity \( \mathbf{U} \) at the boundary \( \Gamma \). The fundamental solution for this linear operator is obtained from

\[
\overline{D} \nabla^2 G + \mathbf{U} \cdot \nabla G + \delta(p, \zeta) = 0 
\]

(13)

For the 2D case,

\[
G = \frac{1}{2\pi \overline{D}} K_0(\mu r) \exp \left( -\frac{\mathbf{U} \cdot \mathbf{r}}{2\overline{D}} \right) 
\]

(14a)

\[
G^* = \frac{1}{2\pi \overline{D}r^2} \left[ \mu \eta r K_1(\mu r) - \frac{U_n r^2}{2\overline{D}} K_0(\mu r) \right] \exp \left( -\frac{\mathbf{U} \cdot \mathbf{r}}{2\overline{D}} \right) 
\]

(14b)

and for the 3D case,

\[
G = \frac{1}{4\pi \overline{D}r} K_0(\mu r) \exp \left( -\frac{(U \cdot r + Vr)}{2\overline{D}} \right) 
\]

(15a)

\[
G^* = -\frac{1}{4\pi \overline{D}r^3} \left[ \eta Vr + \frac{U_n r^2}{2\overline{D}} \right] \exp \left( -\frac{\mathbf{U} \cdot \mathbf{r} + Vr}{2\overline{D}} \right) 
\]

(15b)

where \( \mu = V/(2\overline{D}) \) and \( V = |\mathbf{U}| \). Some of the investigators who have used the fundamental solution based on the EDC equation are Skerget et al. [24] and Ikeuchi and Onishi [25]. In this chapter, the computer model that is based on the elliptic diffusion–convection operator is referred to as EDC.

### 2.3 Formulation with the transient diffusion (TD) operator

This formulation uses the temporal derivative term in conjunction with the diffusion term of eqn (1). It is based on a form of eqn (1) that is given by

\[
\overline{D} \nabla^2 c - \frac{\partial c}{\partial t} = b 
\]

(16)

where the pseudo-forcing term \( b \) accounts for the convective and source terms

\[
b = \mathbf{u} \cdot \nabla c + Q 
\]

(17)
The corresponding integral equation arising from applying Green’s identity to eqn (16) is

\[ \lambda(\xi)c(\xi)^2 + \int_0^\Delta t \int_\Gamma \left[ G^*(r, \tau)c - G(r, \tau) \frac{\partial c}{\partial n} \right] d\tau ds - \int_\Omega G(r, \Delta t)c^{(1)} dA + \int_0^\Delta t \int_\Omega bG(r, \tau) d\tau dA = 0 \] (18)

where the bracketed superscripts 1 and 2, respectively, denote the previous time level \( t_1 \) and the current time level \( t_2 \). The fundamental solution is the solution in an infinite spatial region of

\[ \mathcal{D}^2 G + \frac{\partial G}{\partial \tau} + \delta(r, \tau) = 0 \] (19)

that is given by

\[ G = \frac{H(\tau)}{4\pi D_\tau^{|k/2|}} \exp \left( -\frac{r^2}{4D\tau} \right) \] (20a)

\[ G^* = -\frac{\eta}{2D\tau} G \] (20b)

where \( k \) equals the number of spatial dimensions of the problem. The expression for the normal derivative of the fundamental solution can be inserted into eqn (18) to yield

\[ \lambda(\xi)c(\xi)^2 - \int_0^\Delta t \int_\Gamma G(r, \tau) \left( \frac{\eta}{2\tau} c + \mathcal{D} \frac{\partial c}{\partial n} \right) d\tau ds - \int_\Omega G(r, \Delta t)c^{(1)} dA + \int_0^\Delta t \int_\Omega bG(r, \tau) d\tau dA = 0 \] (21)

It should be noted that domain integration of the initial data is still required in this formulation. Some of the investigators who have used the fundamental solution of eqn (20a) are Taigbenu and Liggett [15], Zabaras and Mukherjee [26], and Young et al. [27, 28]. Young and his coworkers incorporated the method of characteristics into the formulation when solving the vorticity transport equation. The solutions from the computer model based on the transient diffusion operator are referred to as TD in this chapter.

2.4 Formulation with the transient diffusion–convection (TDC) operator

This formulation uses the temporal derivative term in conjunction with the homogeneous diffusion–convection terms of eqn (1). Because the fundamental solution can only be derived with constant coefficients and a uniform velocity field, the
velocity in the convective term is split in the same manner as done earlier for the EDC formulation. The linear form of eqn (1) that is used is given by

$$\overline{D} \nabla^2 c - \mathbf{U} \cdot \nabla c - \frac{\partial c}{\partial t} = b$$

(22)

where the pseudo-force term $b$ accounts for the heterogeneous convective and source terms.

$$b = \hat{\mathbf{u}} \cdot \nabla c + Q$$

(23)

The corresponding integral equation arising from applying Green’s identity to eqn (22) is

$$\lambda(\zeta) c(\zeta) + \int_0^{\Delta t} \int \left[ G^*(r, \tau) c - G(r, \tau) \frac{\partial c}{\partial n} \right] \, d\tau \, ds$$

$$+ U_n \int_0^{\Delta t} \int \frac{1}{2} \left[ \eta \tau + U_n \right] c + \int_0^{\Delta t} \int bG(r, \tau) \, d\tau \, dA = 0$$

(24)

The fundamental solution is the solution in an infinite spatial region of

$$\overline{D} \nabla^2 G + \mathbf{U} \cdot \nabla G + \frac{\partial G}{\partial \tau} + \delta(r, \tau) = 0$$

(25)

It is given by

$$G = \frac{H(\tau)}{[4\pi \overline{D} \tau]^{k/2}} \exp \left[ - \left( \frac{\tau V^2}{4\overline{D}} + \frac{r^2}{4\overline{D} \tau} + \frac{\mathbf{U} \cdot \mathbf{r}}{2\overline{D}} \right) \right]$$

(26a)

$$G^* = -\frac{1}{2\overline{D}} \left( \frac{\eta}{\tau} + U_n \right) G$$

(26b)

where $k$ equals the number of spatial dimensions of the problem and, as in the nontransient version of this formulation, $V = |\mathbf{U}|$. Inserting the expression for the normal derivative of the fundamental solution into eqn (24) simplifies the integral equation to

$$\lambda(\zeta)c(\zeta) + \int_0^{\Delta t} \int G(r, \tau) \left[ \frac{1}{2} \left( \frac{\eta}{\tau} - U_n \right) c + \overline{D} \frac{\partial c}{\partial n} \right] \, d\tau \, ds$$

$$- \int_0^{\Delta t} \int G(r, \tau) c^{(1)} dA + \int_0^{\Delta t} \int bG(r, \tau) \, d\tau \, dA = 0$$

(27)

It should be noted that domain integration of the initial data is also required in this formulation. Taigbenu [29] and Kakuda and Tosaka [30] used this fundamental
solution of eqn (26a) to solve diffusion–convection problems in one spatial dimension. In this chapter, the solutions from the computer model based on the transient diffusion–convection operator are referred to as TDC.

The choice of formulation or linear differential operator adopted has largely depended on the personal inclinations of investigators. However, some general statements can be made concerning these formulations. The expressions of the fundamental solutions with the time variable tend to be more complicated than those without it. Their complicated expressions extend to the calculations of the integrations over elements so that more computational effort is generally required in evaluating the elements of the global coefficient matrix. A number of the integrations cannot be carried out analytically, and so have to be evaluated numerically. One disadvantage of the formulations that are based on nontransient fundamental solutions is that the temporal derivative has to be approximated by a finite difference expression. That provides some limit on the size of the time step that can be taken to ensure that the numerical scheme remains stable.

3 Numerical implementation

The numerical implementation of the integral equations requires that the boundary and, sometimes, the domain be discretized into suitable elements and functional quantities be allowed to vary over those elements using some prescribed interpolation functions. The order of polynomial used as the interpolation function bears a close correlation to the computational effort involved in evaluating the element integrations. Zero and first order polynomials are commonly used as interpolation functions. For the boundary integrations, line segments or plane surfaces are commonly used in discretizing the boundary, while spline elements have occasionally been used. Over a typical element, functional quantities are interpolated according to the relationship

\[ c(r, t) \approx N_i(r)c_i(t) \]  

(28)

where \( N_i \) is the interpolation function with respect to the nodal point \( i \).

A number of approaches have evolved in the numerical implementation of the integral equation. They have arisen largely because of the domain integrals that contain the initial data distribution and nonhomogeneous transport terms. The classical approach gives rise to a solution scheme in which the solution at any node is obtained from contributions from all the nodes in the computational region. For that reason, the coefficient matrix is always dense and fully populated (Fig. 1a). For large-scale regional transport problems, this could require an enormous amount of computing resources if the matrix has to be decomposed at each time step. In this age of vector and parallel computing, that is not too great a challenge to handle.

In the classical approach, the evaluation of the domain integrations requires that the region be discretized into suitable polygonal elements so that some measure of accuracy is achieved in describing the distribution of the dependent variable over the elements. That makes BEM quite unattractive in the sense that its computational advantage as a boundary-only method is lost.
Figure 1: Typical forms of the coefficient matrix: (a) fully populated with single domain; (b) partial domain discretization; (c) full domain discretization.

In the classical approach, the outcome of implementing the boundary and domain integrations gives rise to a matrix equation that takes, for the ED and EDC formulations that use nontransient fundamental solutions, the form

$$B_{ij}c_j + H_{ij} \varphi_j + T_{ij} \frac{dc_j}{dt} = S_i$$

and, for the TD and TDC formulations that use transient fundamental solutions, the form

$$B_{ij}c_j^{(2)} + H_{ij} \varphi_j^{(2)} = S_i$$

where $\varphi = \frac{dc}{dn}$. It should be understood that the labels of the matrices in eqns (29a) and (29b) have been used in a generic sense, without implying that their elements are the same for the four different formulations. The vector $S_i$ is a known vector, in eqn (29a), accounts for known sources while, in eqn (29b), accounts for known sources and data on $c$ and $\varphi$ at the previous time $t_1$.

The matrix equation (29a) from the ED and EDC formulations can be solved only after the temporal derivative is discretized. This is done by finite differencing, i.e.

$$\frac{dc}{dt} \approx \frac{c^{(2)} - c^{(1)}}{\Delta t}$$

This simplification allows for the introduction of a difference weighting factor $\alpha$ that takes a value of between zero and unity. The weighting factor is used to weight the other terms in eqn (29a) so as to reflect the time within the time step $\Delta t$ at which differencing is done. An $\alpha$ value of zero indicates that differencing is done at $t_1$,
while a value of unity indicates that differencing is done at \( t_2 \). The introduction of eqn (30) into eqn (29a) yields

\[
\left( \alpha B_{ij} + \frac{T_{ij}}{\Delta t} \right) c_j^{(2)} + \alpha H_{ij}\psi_j^{(2)} = R_i
\]

(31)

where \( R_i = [\beta B_{ij} + T_{ij}/\Delta t] c_j^{(1)} + \beta H_{ij}\phi_j^{(1)} \) and \( \beta = \alpha - 1 \). Equation (31) for the ED and EDC formulations, now in a similar form as eqn (29b) for the TD and TDC formulations, can be solved after effecting the known boundary conditions. The resultant matrix equation for all the formulations has the form

\[
A_{ij}h_j^{(2)} = P_i
\]

(32)

where \( h = [c, \phi]^T \) is a mixed vector of unknowns. In the classical approach, the global coefficient \( A_{ij} \) is dense and fully populated.

### 3.1 Dual reciprocity method

In the classical approach, domain integrations are implemented usually by Gauss quadrature methods. However, to still retain the boundary-only character of BEM, a number of initiatives have been pursued [17, 31]. The most notable one is the DRM that was first initiated by Nardini and Brebbia. It transforms these domain integrals into surface integrals by making use of radial basis functions. Though domain integrals are avoided using the DRM, it nonetheless still requires that some number of nodes be chosen within the computational region. The DRM is well documented in many works by Brebbia and his co-workers [17, 23, 32]. Here, it is only briefly described to ensure completeness of the chapter, and readers are directed to a more detailed discussion of the method in the references provided. We shall focus only on the domain integration term given as \( \int_{\Omega} bGdA \). The basic idea of the DRM is to express \( b \) in terms of radial interpolation functions, i.e.

\[
b(r, t) \approx \sum_{j=1}^{M} \omega_k(t)f_k(r)
\]

(33)

where \( f_k(r) \) are the radial interpolation functions, \( M \) is the number of nodal points at which interpolation is carried out, and \( \omega_k \) are unknown coefficients. There are a number of such functions that can be used of which the one based on the distance vector between the field and the source node is most widely used, i.e. \( f_k(r) = 1 + r \). A new auxiliary function \( \omega_k \) is proposed such that its Laplacian equals the radial interpolation function, i.e. \( \nabla^2 \psi_k = f_k \). To this, Green’s identity is applied to yield an equation that is similar to eqn (6)

\[
\int_{\Omega} f_k GdA = -\lambda(\xi)\psi_k(\xi) - \int_{\Gamma} \left[ \psi_k G^* - G \frac{\partial \psi}{\partial n} \right] ds
\]

(34)
Using all $M$ radial functions $f_k$ in eqn (33), the expression for the domain integral now becomes

$$\int \int_{\Omega} bGdA = \sum_{k=1}^{M} \omega_k \left( -\lambda(\zeta)\psi_k(\zeta) - \int_{\Gamma} \left[ \psi_k G^* - G \frac{\partial \psi_k}{\partial n} \right] ds \right)$$  \hspace{1cm} (35)$$

Now the domain integration involves only boundary integrals. It has been achieved by applying the reciprocity principle used for the ED operator, hence, the name DRM. The unknown coefficients $\omega_k$ are obtained by inversion of eqn (33) at the $M$ nodal points, i.e.

$$\omega = F^{-1}b$$  \hspace{1cm} (36)$$

### 3.2 The Green element method

All boundary element implementing procedures so far applied to the diffusion–convection transport equation can be considered to fall within a spectrum of formulations with meshless formulations at one end and, on the other, full domain decomposition formulations to which the DRM belongs. Meshless formulations, which the DRM attempts to achieve, are bound to do well only for weakly domain-dominant problems (weak nonhomogeneity and nonlinearities), but their numerical appeal lies in the retention of the original spirit of BEM. Domain decomposition formulations, on the other hand, hold the key in solving highly domain-dominant problems to which the diffusion–convection transport equation belongs. However, they tend to have less appeal because they conjure the FEM which the BEM sought to overcome in the first instance.

Domain decomposition was originally proposed to allow the BEM to handle large field problems by decomposing the original domain into subdomains within which the integral equation is applied, while imposing the appropriate compatibility relations at the interfaces of adjacent subdomains. Whereas fully populated matrices are encountered in BEM matrices with single-domain formulations (Fig. 1a), those with domain decomposition result in block-banded matrices with the blocks of adjacent domains overlapping themselves (Fig. 1b). The solution of the global coefficient matrix from these domain discretization schemes cannot be effected because the system is generally overdeterminate. Several schemes are used to reduce the overdeterminate system to a closed system that can then be solved [20]. The GEM is not primarily motivated only by the achievement of a banded matrix (Fig. 1c), but by the ease and flexibility that the approach offers in evaluating the domain integrations. This latter numerical feature stems from the fact that when evaluating the domain integrations, the source and field nodes always share the same element, while the flexibility allows for heterogeneous and nonlinear terms to be correctly represented from element to element. It is this that has made it possible for the calculation of the convection–diffusion problems with heterogeneous parameters and reaction terms.

The GEM essentially calculates the integral equation earlier obtained in an element or cell, and obtains the global coefficient matrix by aggregating the element...
equations for all the elements. The aggregation is done such that compatibility conditions at inter-element boundaries are applied and \( \partial c/\partial n \) is expressed in terms of \( c \), so that the outcome is that the solution for \( c \) is calculated at all nodes, and \( \partial c/\partial n \) at the external nodes. Details of the method can be found in references [21] and [22]. Popov and Power [23] have incorporated DRM into GEM so that domain integrations are avoided.

4 Numerical stability for homogeneous diffusion–convection

BEM schemes for the diffusion–convection equation are generally time-marching in nature, and numerical stability analysis provides an insight into how errors arising from the discrete replication of the original differential equation and computer precision propagate in both amplitude and speed with time. The stability of the ED, TD, and TDC formulations are examined for homogeneous transport in one dimension, i.e. \( \partial c/\partial n \). The boundary element coefficients from the three formulations using linear interpolating functions in space and time take the form of eqn (29b)

\[
B_{ij}^{c(2)} + H_{ij}^{c(2)} = S_i
\] (37)

Since there is no source term, the known vector on the right-hand side of eqn (37) essentially accounts for known data at the previous time \( t_1 \). Essentially the three models are time-marching schemes which use the known data at the beginning of the time step to obtain their new values at the end of the time step on the basis of the numerical replication of the differential equation. For a well-posed initial-value problem, the solution at any time level is expected to be bounded, and this can only be achieved by a numerical scheme which does not allow the solution and accumulated computational errors to grow out of bounds.

The stability characteristics of the three formulations are assessed by the method of Stone and Brian [33], which has been applied by Leendertse [34, 35], Gray and Pinder [8], Gray and Lynch [36], and Taigbenu [37, 38]. It represents the general solution of the linear differential equation by an infinite series of Fourier wave components, and the stability characteristics of the numerical scheme are assessed by comparing the numerical amplitude and speed of each wave component to their theoretical values. A scheme is said to be dissipative if it is unable to correctly reproduce the amplitude of the Fourier wave component, and it is dispersive if it is unable to correctly reproduce its speed. Dissipative schemes cause steep gradients in the solution to become smeared, while dispersive schemes cause the small wavelengths to be out of phase with the longer wavelengths which usually manifest as oscillations in the numerical solution.

The proposed Fourier series solution is

\[
c(x,t) = \sum_{m=-\infty}^{\infty} \Phi_m \exp[i(\sigma_m x + \beta_m t)]
\] (38)

in which, for each Fourier wave component, \( \beta_m = 2\pi/T_m \) is the temporal frequency, \( T_m \) is the period, \( \sigma_m = 2\pi/L_m \) is the spatial frequency or wave number,
Let $L_m$ be the wavelength, and $\hat{\imath}$ is the imaginary representation of a complex variable. Only one term of the series needs to be examined since the differential operator is linear. The dispersion relationship: $\beta = \sigma (iD\sigma - U)$ is introduced into eqn (38) to have for one term of the series solution

$$c = c^{(1)} = \Phi \exp(i\sigma (x - U t)) \exp(-D\sigma^2 t)$$

(39)

Equation (39) indicates that each Fourier wave component is a translatory wave with propagation speed of $U$, and amplitude modification of $\exp(-D\sigma^2 t)$ after an elapse time $\Delta t$. In other words: $c^{(2)} = a_ne^{i\phi}$, where $a_n$ is the theoretical amplification of each Fourier wave after one time step. It has a magnitude of $|a_n| = \exp(-D\sigma^2 \Delta t)$ and phase angle of $\theta_n = -\sigma U \Delta t$. Denoting the magnitude and phase angle of the numerical amplification as $a_n$ and $\theta_n$, respectively, the amplification factor after one wavelength of propagation is

$$T = \left| \frac{a_n}{a_1} \right| = \left( \frac{|a_n|}{\exp(-D\sigma^2 \Delta t)} \right)^N_t = \left( \frac{P_eL^2|a_n|}{\exp(-4\pi^2 C_e^2x^2)} \right)^N_t$$

(40)

where $N_t = L/(\Delta x C_t)$ is the number of time steps for the wave to traverse one wavelength, $C_t = U\Delta t/\Delta x$ is the element Courant number, and $P_e = U/\Delta x/D$ is the element Peclet number. The corresponding expression for the phase lag at the end of one wavelength of propagation is

$$\Theta = 2\pi \left( \frac{\theta_n}{\theta_1} - 1 \right) = 2\pi \left( \frac{\theta_n}{\sigma \Delta x C_t} - 1 \right)$$

(41)

To evaluate $T$ and $\Theta$ for the three numerical formulations, we consider a computational region that is discretized uniformly by linear elements each of which has a length of $\Delta x$ such that a node of interest $x_i$ is sandwiched between two nodes $x_{i-1}$ and $x_{i+1}$. The numerical scheme modifies $c$ according to the relationship: $c^{(2)} = a_n e^{i\phi}$, and similarly for $\psi$, where $a_n$ is the numerical amplification. Applying the element integral equation (37) to the two elements: $[x_{i-1},x_i]$ and $[x_i,x_{i+1}]$ produces a quadratic equation in $a_n$ that depends on the coefficients $B_{ij}$ and $H_{ij}$ from which the two roots are calculated, though one of them is inadmissible.

For values of $C_t = 0.2$ and $C_t = 1$, $P_e = 2$ and $P_e = 50$, the propagation characteristics of the ED, TD, and TDC formulations are compared. The first sets of results, shown in Fig. 2a–d, give the variation of $|a_n|$ with respect to $L/\Delta x$ and they indicate that all three formulations are stable. The next sets of plots compare the numerical amplification values to their corresponding theoretical values, i.e. the variation of $T$ and $\Theta$. Ideally $T$ should be unity and $\Theta$ zero.

These plots for $C_t = 0.2$ and $P_e = 2$, are in Fig. 3a and b, in Fig. 4a and b for $C_t = 1$ and $P_e = 2$, in Fig. 5a and b for $C_t = 0.2$ and $P_e = 50$, and in Fig. 6a and b for $C_t = 1$ and $P_e = 50$. The results show that at small values of $C_t$ and $P_e$, the ED formulation with $\alpha = 0.5$ (Crank–Nicholson scheme) and the TDC formulation exhibit the least phase lag, but the latter is more dissipative (Fig. 3a and b). (The harmonics are considered to be correctly propagated when the amplification factor is within 5%...
of unity and the phase angle shift is within 5%.) When the value of the Courant number is increased to unity for small values of the Peclet number (diffusion-dominant transport), the propagation characteristics of the Fourier harmonics by the numerical schemes become slightly different (Fig. 4a and b). Only harmonics with
wavelengths larger than four times the spatial element size are correctly propagated in speed by the ED \((\alpha = 0.5)\) and TDC formulations. The amplitudes of the wave components are damped more by the TD and TDC formulations than by the ED formulation. In contrast to the case when \(C_r = 0.2\), all ED schemes amplify the amplitudes of the short wavelengths. What can be considered surprising is the result that the TD and TDC formulations do better in propagating the harmonics at larger values of the Courant number (larger time step) than at smaller values (smaller time step).

When \(C_r = 0.2\) and \(P_e = 50\), the ED formulation with \(\alpha = 0.5\) does best in propagating all harmonics with wavelengths larger than four times the element size (Fig. 5a and b). At this large Peclet number (convection-dominant transport)
and small Courant number, the TD and TDC formulations damp the amplitudes of virtually all harmonics and only correctly propagate the speed of harmonics with large wavelengths 10 times the element size. For this large Peclet number, increasing the Courant number to unity does bring about improvement in the propagating characteristics of the TD and TDC formulations, but the converse is the case with the ED formulation (Fig. 6a and b). The above results are summarized as follows: (1) incorporating the Crank–Nicholson scheme into the ED model gives optimal stability characteristics at small values of the Courant number for all transport modes; (2) the stability characteristics of the TD and TDC are improved when a value of unity is used for the Courant number.

5 Numerical examples of diffusion–convection problems

The ED, TD, and TDC formulations are applied to five examples of transient diffusion–advection transport. The first four examples are one-dimensional in space, while the fifth is two-dimensional.

5.1 Example 1

This first example is the classical 1D transport problem which finds use in evaluating the performance of many numerical schemes. The velocity field is uniform and there are no sources. The boundary and initial conditions are: \( c(0, t > 0) = 1 \), \( \partial c / \partial x \) at \( x = \infty \), \( t > 0 \) = 0, and \( c(x, t = 0) = 0 \); its well-known solution was provided by Ogata and Banks [39]. For \( P_e = 2 \) (diffusion-dominant transport) all the numerical schemes exhibit negligible spurious oscillations. The breakthrough concentration curves of the exact and numerical solutions at \( t = 0.5 \) are presented in Fig. 7a. The solutions of the TD and TDC formulations are presented when \( C_r = 1 \) and small Courant number, the TD and TDC formulations damp the amplitudes of virtually all harmonics and only correctly propagate the speed of harmonics with large wavelengths 10 times the element size. For this large Peclet number, increasing the Courant number to unity does bring about improvement in the propagating characteristics of the TD and TDC formulations, but the converse is the case with the ED formulation (Fig. 6a and b). The above results are summarized as follows: (1) incorporating the Crank–Nicholson scheme into the ED model gives optimal stability characteristics at small values of the Courant number for all transport modes; (2) the stability characteristics of the TD and TDC are improved when a value of unity is used for the Courant number.

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because both formulations do better at this Courant value than at \( C_r = 0.2 \). The ED solution is obtained with \( C_r = 0.2 \). All three formulations are able to correctly reproduce the breakthrough curve which is not steep because of diffusion dominance. For the strong advection-dominant transport (\( Pe = 50 \)), the TDC model does not exhibit any oscillations that are exhibited by the ED and TD models (Fig. 7b). All the models are able to capture the steep front of the breakthrough curve.

5.2 Example 2

This second example is that of an initial Gauss-hill concentration profile subjected to dispersion and uniform advection. The boundary conditions and initial Gauss-hill profile are: \( c(x = -\infty, \ t) = 0 \), \( \partial c(x = \infty, \ t)/\partial x = 0 \), and \( c(x, \ 0) = \exp[-(x-x_0)^2/2\sigma_0^2] \); the exact solution is \( c(x, \ t) = \sigma_0 \exp[-(x-x_0)^2/2\sigma^2]/\sigma \), where \( \sigma^2 = \sigma_0^2 + 2Dt \) and \( x_0 + \int_0^t U(s) \, ds \). Our calculations use \( x_0 = 0 \) and \( \sigma_0 = 0.1 \) to obtain solutions at \( t = 0.5 \). The concentration breakthrough curves at \( t = 0.5 \) can be found in Fig. 8a and b. They are obtained for the diffusion-dominant transport (\( Pe = 2 \)) and convection-dominant transport (\( Pe = 50 \)). As in the previous example, a value of \( C_r = 0.2 \) is used in the ED model with the Crank–Nicholson scheme, while unit value of the Courant number is used in the TD and TDC models. None of numerical models exhibit any significant oscillations or wiggles upstream or downstream of the concentration hill, but the ED model does indicate superior performance in terms of being able to accurately model the concentration hill.

5.3 Example 3

The third example is that of a contaminated stream subjected to advection from a freshwater source and biological/chemical degradation. The initial and boundary
conditions are: $c(x, t = 0) = 1, c(x = 0, t > 0) = 0$, and $\partial c (x = \infty, t > 0)/\partial x = 0$. The exact solution is given by van Genuchten and Alves [2]. Two cases of this example are examined with the following parameters: the first is $U = 1, D = 0.025,$ and $P_e = 2$, and the second is $U = 1, D = 0.0005$, and $P_e = 50.$

For both cases the source term is a reaction term expressed as $Q = 0.2c$. Only the ED and TD models are applied, and the numerical calculations use a uniform spatial element size of 0.025. The numerical and exact solutions, obtained at times 0.5 and 1.0, are presented in Fig. 9a for the first case, while those of the second case are presented in Fig. 9b. For both cases, the ED model reproduced the exact solution more closely than the TD model. The numerical solutions have trailing oscillations for the strong convection-dominant transport but their strength appears to decrease as simulation time increases.
5.4 Example 4

This example is the case of transport of an initial concentration profile of unit value everywhere in a uniform flow field \( U \) in the \( x \) direction. The boundary conditions are \( c(x=0, t>0) = 0 \) and \( c(x=1, t>0) = 0 \). The exact solution to this problem can be found in reference [19]. Twenty uniform rectangular elements are used to discretize the domain, while the time step employed in the numerical calculations is expressed in terms of the Courant number. These values are: 0.1, 0.25, and 0.5. The results of the ED model with \( C_r = 0.1 \) and that of the TD model with \( C_r = 0.5 \) are presented in Fig. 10a for \( U = 5 \) and Fig. 10b for \( U = 20 \). The ED solution is slightly superior in approximating the exact solution than the TD model.

5.5 Example 5

This example is a transient transport problem in two dimensions for which Cleary [1] derived an exact solution. The pollutant, which is continuously injected into the flow medium from a line source, is dispersed in the longitudinal and transverse directions and advected by a uniform velocity field along the longitudinal direction. At the initial time, the concentration has zero value everywhere. The boundary conditions for this example are:

\[
c(0, y, t) = 1, \quad 2 \leq y \leq 3; \quad c(0, y, t) = 0, \quad 0 \leq y < 2 \quad \text{and} \quad 3 < y \leq 5 \quad (42a)
\]

\[
\frac{\partial c(x, 0, t)}{\partial y} = \frac{\partial c(x, 5, t)}{\partial y} = 0, \quad x > 0; \quad \frac{\partial c(\infty, y, t)}{\partial x} = 0, \quad 0 \leq y \leq 5 \quad (42b)
\]

Finite element simulations of this example were carried out by Yeh [40], and the parameters employed in those simulations are also used here. Although the domain is semi-infinite, a finite domain of \( 15 \times 2.5 \), which is discretized into 150 uniform
rectangular elements each of $0.5 \times 0.5$, is used for the calculations. Following Yeh [40], three transport modes are examined: the case of diffusion-dominant transport ($P_e = 0.05$), equal dominance of diffusion and convection ($P_e = 1$), and the convection-dominant transport ($P_e = 50$). A uniform time step of 0.2 is employed in all the calculations, and the breakthrough concentration fronts at $t = 4$ along $y = 2.5$ are presented in Fig. 11a–c for the three cases. The finite element solutions are obtained by an orthogonal weighting scheme. For all three cases, the ED formulation reproduces the concentration front better than the TD formulation or the FEM. For lower values of the Peclet number, the solutions from the current formulation are about the same as the FEM solutions, while for the advection-dominant transport, the TD formulation is dissipative with a smeared front and the FEM is both dissipative and dispersive with the concentration shooting higher than the exact value at the upstream end of the front.

6 Burgers’ equation

Burgers’ equation [41, 42] is a second-order simplification of the momentum transport equation or the Navier–Stokes equation, and it provides a useful model for
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flow phenomena in which there exist the balancing effects of viscous and inertia or convective forces. Its unique features of a propagating wave front when inertia is dominant, and a stretched wave front when viscous forces are pronounced make the solution of Burgers’ equation quite a challenge. Exact solutions of the equation have been obtained mostly for infinite domains by the Cole–Hopf transformation [42, 43], and are summarized by Benton and Platzman [44].

A subdomain discretization of the integral equation in the Green element sense is used to solve the Burgers’ equation. Three formulations are applied; these are the ED, TD, and TDC formulations. The discretized integral equations are nonlinear, and they are linearized by either the Newton–Raphson or Picard algorithm. The efficiency and accuracy of the three formulations are evaluated with three numerical examples.

7 Numerical formulations of Burgers’ equation

The mathematical statement that describes one-dimensional nonlinear fluid flow phenomenon of shock or wave propagation with viscous dissipation, widely known as the Burgers’ equation, is given by Lighthill [45]

$$D \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} = 0 \quad \text{on } x_0 \leq x \leq x_L$$

in which $D = 1/R_e$ is the reciprocal of the flow Reynolds number which is a dimensionless parameter that gives the relative magnitude of inertia forces to viscous forces, and $u(x, t)$ is the dependent variable which denotes the velocity field. Fletcher [46] discussed the important features of eqn (43) as a prototype of the force balance between the nonlinear acceleration or inertia or convective term $u \partial u/\partial x$ and the diffusive term $D \partial^2 u/\partial x^2$. All three numerical formulations follow a unified approach of (1) constructing the Green’s function to an appropriate linear differential operator of the flow equation, (2) employing Green’s second identity in transforming the flow equation into an integral one, (3) discretizing the integral equation by suitable elements to obtain a system of discrete equations, and (4) linearizing the nonlinear discrete equations either by the Newton–Raphson or Picard algorithm.

7.1 ED formulation for Burgers’ equation

The ED formulation derives its fundamental solution from the second-order diffusion term: $d^2G/\partial x^2 + \delta(x - \zeta) = 0$, where $G = -|x - \zeta|/2$. Applying Green’s identity to the differential equation yields the integral equation for a typical linear element $[x_1, x_2]$

$$D \left( \lambda(\zeta)u(\zeta, t) + [G^2 u]_{x_1}^{x_2} - [G\phi]_{x_1}^{x_2} \right) + \int_{x_1}^{x_2} bGdx = 0$$

(44)
in which \( b = u \partial u / \partial x + \partial u / \partial t \) and \( \psi \equiv \partial u / \partial x \). The line integral of eqn (44) is evaluated by approximating \( u \) and \( \psi \) with linear interpolation functions \( N_j \), i.e.

\[
D \left( \lambda u_i + \left[ G^* u \right]_{x_1}^{x_2} - \left[ G \psi \right]_{x_1}^{x_2} \right) + \int_{x_1}^{x_2} G \left( N_j N_i u j \psi + N_j \frac{du}{dt} \right) \, dx = 0 \tag{45}
\]

or in matrix form

\[
B_{ij} u_j + H_{ij}(u) \psi_j + T_{ij} \frac{du}{dt} = S_i \tag{46}
\]

where

\[
B_{ij} = D \left( \frac{1}{2} \delta_{ij} + G^*(x_2 - x_i) \delta_{ij} - G^*(x_1 - x_i) \delta_{ij} \right) \tag{47a}
\]

\[
H_{ij} = -D(G(x_2 - x_i) \delta_{ij} - G(x_1 - x_i) \delta_{ij}) + \int_{x_1}^{x_2} G N_j N_i u_j dx \tag{47b}
\]

\[
T_{ij} = \int_{x_1}^{x_2} G N_j dx \tag{47c}
\]

Details of the expressions of these matrices can be found in reference [47]. It should be noted that the matrix \( H_{ij} \) depends on the velocity field, hence, the nonlinear nature of the discrete equations. Using the same time discretization described earlier in Section 3, eqn (46) becomes similar to eqn (31), i.e.

\[
\left( \alpha B_{ij} + \frac{T_{ij}}{\Delta t} \right) u_j^{(2)} + \alpha H_{ij} \psi_j^{(2)} - R_i = g_i \tag{48}
\]

Denoting \( h = (u, \psi)^T \) as the mixed solution vector, the N–R algorithm for eqn (48) refines an estimate of the solution \( h^{(2,m)} \) by the relationship \( h^{(2,m+1)} = h^{(2,m)} + \Delta h^{(2,m+1)} \), where \( m \) is the iteration number and \( \Delta h^{(2,m+1)} \) is the increment that is obtained from:

\[
j_{ij}^{(2,m+1)} = -g_i^{(2,m)} \tag{49}
\]

in which the Jacobian \( j_{ij}^{(2,m)} \) takes the expression

\[
j_{ij}^{(2,m)} = \left\{ \begin{array}{l}
\frac{\partial g_i}{\partial u_j} \left| _{u_j = u_j^{(2,m)}} \right. = \alpha \left[ B_{ij} + \frac{dH_{ik}}{du_j} \psi_k^{(2,m)} \right] + \frac{T_{ij}}{\Delta t} , \\
\frac{\partial g_i}{\partial \psi_j} \left| _{\psi_j = \psi_j^{(2,m)}} \right. = \alpha H_{ij}
\end{array} \right. \tag{50}
\]

Equation (49) is solved at each time step until convergence is achieved.
7.2 TD formulation for Burgers’ equation

The TD formulation uses the fundamental solution $G(x, \tau) = H(\tau) \exp[-x^2/4D\tau]/\sqrt{4\pi D\tau}$ to the linear diffusion equation $D\partial^2 G/\partial x^2 + \partial G/\partial \tau + \delta(x, \tau) = 0$. The integral equation presented earlier in eqn (21) is applied to a typical spatial element $[x_1, x_2]$ in time interval $[t_1, t_2]$

$$\lambda u_j^{(2)} + \int_0^{\Delta t} D \left[ G(x_2, \tau) \delta_{2j} - G(x_1, \tau) \delta_{1j} \right] d\tau - \int_{x_1}^{x_2} G(x, \Delta \tau) u^{(1)} \, dx$$

$$+ \int_0^{\Delta t} \int_{x_1}^{x_2} G(x, \tau) u \varphi \, dx \, d\tau = 0$$

(51)

A linear distribution is prescribed for $u$ and $\varphi$ within the spatial element $[x_1, x_2]$ and the temporal element $[t_1, t_2]$, while the convective term is approximated as $\bar{u} \varphi$, where $\bar{u}$ is the average velocity within the element. With this approximation, eqn (51) in matrix form becomes

$$B_{ij} u_j^{(2)} + H_{ij} (\bar{u}) \varphi_j^{(2)} = S_i$$

(52)

where

$$B_{ij} = \frac{1}{2} \delta_{ij} + D \int_0^{\Delta t} \frac{\tau}{\Delta t} \left[ G^*(x_2 - x_i, \tau) \delta_{2j} - G^*(x_1 - x_i, \tau) \delta_{1j} \right] d\tau$$

(53a)

$$H_{ij} = -D \int_0^{\Delta t} \frac{\tau}{\Delta t} \left[ G(x_2 - x_i, \tau) \delta_{2j} - G(x_1 - x_i, \tau) \delta_{1j} \right] d\tau$$

$$+ \bar{u} \int_0^{\Delta t} \int_{x_1}^{x_2} \frac{\tau}{\Delta t} G(x - x_i, \tau) N_j \, dx \, d\tau$$

(53b)

$$S_i = -\left\{ D \int_0^{\Delta t} \left( 1 - \frac{\tau}{\Delta t} \right) \left[ G^*(x_2 - x_i, \tau) \delta_{2j} - G^*(x_1 - x_i, \tau) \delta_{1j} \right] d\tau$$

$$- G(x - x_i, \Delta t) N_j \, dx \right\} u_j^{(1)} - \left[ D \int_0^{\Delta t} \left( 1 - \frac{\tau}{\Delta t} \right) \left[ G(x_2 - x_i, \tau) \delta_{2j} - G(x_1 - x_i, \tau) \delta_{1j} \right] d\tau$$

$$- G(x_1 - x_i, \tau) \delta_{1j} \right\} d\tau - \bar{u} \int_0^{\Delta t} \int_{x_1}^{x_2} \left( 1 - \frac{\tau}{\Delta t} \right) G(x - x_i, \tau) N_j \, dx \, d\tau \right\} \varphi_j^{(1)} \right\}$$

(53c)
The analytical expressions for these element matrices can be found in reference [22]. Equation (52) is nonlinear, and can be solved by applying a nonlinear solution scheme. Using the Picard algorithm, the nonlinear discrete eqn (52) is linearized by using known estimates of \( u = u^{(2,m)} \) to calculate \( \bar{u} = \bar{u}^{(m)} \) and, therefore, the right-hand side of eqn (52). The refined estimate of the solution \( h^{(2,m+1)} = [u^{(2,m+1)}, \phi^{(2,m+1)}]^T \), where \( m \) is the iteration, is obtained by solving eqn (52) after incorporating the known boundary conditions. The solution refinement process is continued at each time step until \( |h^{(2,m+1)} - h^{(2,m)}| \) at all nodes fall below a predetermined accuracy tolerance.

### 7.3 TDC formulation for Burgers’ equation

This formulation is based on the 1D version of that presented in Section 2.4. It uses the fundamental solution \( G(x, \tau) = H(\tau) \exp\left[-(x/\sqrt{4D\tau} + \bar{u}/\sqrt{4D})^2\right]/\sqrt{4\pi D\tau} \) to the linear diffusion equation \( D\partial^2 G/\partial x^2 + \bar{u}\partial G/\partial x + \partial G/\partial \tau + \delta(x, \tau) = 0 \). The 1D form of the integral equation (24) is

\[
\lambda u^{(2)}_i + \int_0^{\Delta t} \left( \left( \bar{u} - \chi \right) G_1^2 - D \left( \phi \frac{\partial G}{\partial x} \right) \right) \, d\tau + \int_{x_1}^{x_2} G(x, \Delta t) u^{(1)} \, dx + \int_0^{\Delta t} \left[ Gu \right]_1^2 \, d\tau = 0
\]

(54)

Similar to the approach of Kakuda and Tosaka [30], \( u \) is approximated by linear interpolation functions in space and time, and \( \phi \) by its value at the current time to simplify eqn (54) to

\[
\lambda u^{(2)}_i + \frac{1}{2} \int_0^{\Delta t} \left( \left( \bar{u} - \chi \right) G_1^2 - D \left( \phi \frac{\partial G}{\partial x} \right) \right) \, d\tau - \int_{x_1}^{x_2} G(x, \Delta t) u^{(1)} \, dx = 0
\]

(55)

In eqn (55), we have used the expression for \( G^* = -(x/\tau + \bar{u})G/2D \). In matrix form eqn (55) is

\[
B_{ij}(\bar{u})u^{(2)}_j + H_{ij}(\bar{u})\phi^{(2)}_j = S_i
\]

(56)

where

\[
B_{ij} = \frac{1}{2} \delta_{ij} + D \int_0^{\Delta t} \left( \bar{u} - \chi \right) \frac{\partial G}{\partial x} \frac{\partial G}{\partial x} \, d\tau - \int_{x_1}^{x_2} G(x, \Delta t) \frac{\partial G}{\partial x} \, dx
\]

(57a)

\[
H_{ij} = -D \int_0^{\Delta t} \left[ G(x_2 - x_1, \tau) \delta_{ij} - G(x_1 - x_1, \tau) \delta_{ij} \right] \, d\tau
\]

(57b)
Equation (56) constitutes the system of discrete element equations of the TDC formulation for Burgers’ equation. The expressions for the element matrices can be found in references [30] and [22], and they depend on the value of the primary variable \( u \). The Picard algorithm is employed to linearize the formulation in the same way as for the TD formulation.

8 Numerical examples of Burgers’ equation

The capabilities of the three formulations are demonstrated with three examples. The first two examples have analytic solutions with which we validate the numerical solutions, while the finite element solutions of the third example are used for comparison.

8.1 Example 1 of Burgers’ equation

The first example is an initial sinusoidal wave which is allowed to propagate and diffuse within a confined flow domain in the \( x \)-dimension. The problem has the following boundary conditions:

\[
\begin{align*}
    u(0, t) &= 0, \\
    u(1, t) &= 0 \\
    u(x, t) &= \sin \pi x
\end{align*}
\]  
(58)

The exact solution to this problem, in the form of an infinite series, has been provided by Cole [43]. Using 100 linear elements and a time step of 0.01 in all the numerical calculations, the numerical and exact solutions are presented in Fig. 12a for \( Re = 10^2 \), and in Fig. 12b for \( Re = 10^3 \). In all the numerical calculations, the Crank–Nicholson scheme is used in the ED formulation. The results show that the ED formulation gives the most accurate solution, followed by the TD formulation. The computing times of the ED, TD, and TDC formulations are in the approximate ratio of 2:1:10, with the speed of the TD formulation being enhanced by the ease in the assembly of its global coefficient matrix. The numerical solutions of the velocity profiles, presented in Fig. 12a and b, reflect the general behavior expected of the propagation of the velocity which exhibits a sharp front in the vicinity of \( x = 1 \) at early times, and, as a result of pronounced viscous action in this region, a smeared front at later times. The solution of the ED formulation for \( Re = 10^3 \) in the neighborhood of \( x = 1 \) exhibits oscillations due to its inability to accurately represent the large spatial gradients and incorporate them into the numerical scheme in a stable fashion. However, these oscillations are eliminated by generating the same number of elements with the Chebyshev polynomials so that the nodes cluster in the vicinity of \( x = 1 \).
8.2 Example 2 of Burgers’ equation

The second example is an initial discontinuous wave form which is allowed to diffuse into a continuous wave form, while at the same time being propagated in time along the x-direction. The initial and boundary conditions are given by

\[ u(x, 0) = \begin{cases} 
1, & x \leq 0 \\
0, & x > 0
\end{cases} \]

The exact solution, obtained by the Cole–Hopf transform, is given by Lighthill [45]. The computational domain is discretized into 100 elements and, for the flow with \( R_e = 10 \), a time step of 0.025 is used, while, for \( R_e = 10^2 \), a time step of 0.01 is used. The plots of the numerical and exact solutions are presented in Fig. 13a and b for \( R_e = 10 \) and \( R_e = 10^2 \). Although the flow domain for this example is infinitely extensive, the numerical simulations are carried out using finite domains: 

\(-1.5 \leq x \leq 2.5 \) for the \( R_e = 10 \) and \(-0.7 \leq x \leq 1.3 \) for the case \( R_e = 10^2 \), so that
the exact solutions at the end nodes satisfy the specified boundary conditions at $x = -\infty$ and $x = \infty$ throughout the simulation times.

All the numerical solutions are identical, and that is the reason why only the solutions from one formulation are presented alongside the exact solutions. The $L_2$ norm estimates of the error between the numerical and exact solutions are the same for the three formulations when $Re = 10$, and differ marginally when $Re = 10^2$, as indicated in Fig. 14. That figure shows that the ED formulation is most superior in accuracy, followed by the TD formulation.

8.3 Example 3 of Burgers’ equation

The third example, earlier employed by Varoglu and Finn [48] and Kakuda and Tosaka [30] to verify their numerical solutions, has the following initial and boundary conditions

$$u(x, 0) = \begin{cases} 
1, & x < 5 \\
6 - x, & 5 \leq x \leq 6 \\
0, & x > 6 
\end{cases} \quad (60)$$

$$u(-100, t) = 1, \quad u(20, t) = 0$$
Figure 14: Error plots of numerical schemes of Burgers’ example 2.

Figure 15: Numerical solutions for velocity of Burgers’ example 3.

The solutions of the three formulations for the third example are compared with the finite element solutions of Varoglu and Finn [48] for values of $R_e = 1, 10, \text{ and } 10^2$ in Fig. 15a, b and c, respectively. There is good agreement between the finite element solutions and ED solutions for all three Reynolds number values. However, the TD and TDC formulations produce, for the case $R_e = 10^2$, a velocity front that advances faster than that of the FEM and ED formulations.
9 Conclusion

This chapter has presented some of the computational approaches currently being implemented along the lines of the boundary element theory for the solution of transient diffusion–convection problems. The dual nature of the diffusion–convection equation as a parabolic–hyperbolic equation presents many interesting numerical challenges, especially for convection-dominant transport. Formulations that are based on nontransient and transient fundamental solutions have been applied. The nontransient fundamental solutions tend to be simpler in expression and easier to manipulate when evaluating the boundary and domain integrals. In particular, that based on the ED operator, referred to as the ED formulation in this chapter, has a lot of appeal. Efforts at achieving a boundary-only formulation for the diffusion–convection problem are continuing. The DRM has scored some successes in this direction. However, when applied in the classical manner of implementing BEM, it does not do well for the convection-dominant problem. Implementation of DRM in a Green element sense shows more promising results.

Domain decomposition approaches in implementing the boundary element method arose largely because of the domain integrations that have to be evaluated. Starting from the division of the domain into subdomains that gave rise to block-banded matrices, there are now full domain discretization methods to which the GEM belongs. The GEM has provided additional computational capability of handling heterogeneous and nonlinear transport.

The nonlinear diffusion–convection equation, known as the Burgers’ equation, has also been solved with three boundary element formulations. They are time-marching schemes which update the solution at an earlier time to new values at the current time. The nonlinear nature of the problem requires iteration of the solution to be done at every time level by the three formulations. The ED formulation has an advantage over the other two formulations in terms of accuracy, but uses about twice the computing time of the TD formulation that utilizes the least amount of computing time.

References


Domain Decomposition Techniques for Boundary Elements


