Hybrid numerical methods for convection–diffusion problems in arbitrary geometries

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Abstract

The hybrid nodal-integral/finite element method (NI–FEM) and the hybrid nodal-integral/finite analytic method (NI–FAM) are developed to solve the steady-state, two-dimensional convection–diffusion equation (CDE). The hybrid NI–FAM for the steady-state problem is then extended to solve the more general time-dependent, two-dimensional, CDE. These hybrid coarse mesh methods, unlike the conventional nodal-integral approach, are applicable in arbitrary geometries and maintain the high efficiency of the conventional nodal-integral method (NIM). In steady-state problems, the computational domain for both hybrid methods is discretized using rectangular nodes in the interior of the domain and along vertical and horizontal boundaries, while triangular nodes are used along the boundaries that are not parallel to the x or y axes. In time-dependent problems, the rectangular and triangular nodes become space–time parallelepiped and wedge-shaped nodes, respectively. The difference schemes for the variables on the interfaces of adjacent rectangular/parallelepiped nodes are developed using the conventional NIM. For the triangular nodes in the hybrid NI–FEM, a trial function is written in terms of the edge-averaged concentration of the three edges and made to satisfy the CDE in an integral sense. In the hybrid NI–FAM, the concentration over the triangular/wedge-shaped nodes is represented using a finite analytic approximation, which is based on the analytic solution of the one-dimensional CDE. The difference schemes for both hybrid methods are then developed for the interfaces between the rectangular/parallelepiped and triangular/wedge-shaped nodes by imposing continuity of the flux across the interfaces. A formal derivation of these hybrid methods and numerical results for several test problems are presented and discussed.

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1. Introduction

The convection–diffusion equation (CDE) is used to simulate phenomena in numerous branches of science and engineering, ranging from heat transfer [13] to contaminant transport [11]. Over the years, several methods, including variations of the traditional finite difference and control volume schemes, have been developed to numerically solve the CDE [1,6,16,17,22,28,36]. Furthermore, the exact solution of the CDE in one dimension has been exploited to develop both finite difference-type schemes and finite element methods with exponential or linear-exponential variation between grid points or within cells [4,20,29,37].

Many applications of the CDE require simulations over very large domains. Such simulations if carried out using conventional numerical methods would necessitate a large number of grid points or nodes and hence, large amounts of computer storage, memory, and CPU time. Thus, a numerical scheme that can yield accurate results on a coarse mesh, consisting of fewer nodes or grid points, is desirable.

One such method that fits these requirements quite well is the nodal-integral method (NIM). The NIM is a coarse mesh scheme that relies on a transverse integration step to reduce the governing partial differential equation(s) into a set of ordinary differential equations. The analytical solutions of these ordinary differential equations (or their approximations) are then exploited to derive the necessary algebraic equations that approximate the governing partial differential equation(s). The NIM was initially developed to solve multi-group neutron diffusion equations [14] and the Navier–Stokes equations [2]. Variations of the nodal method, specifically developed for the multi-group neutron diffusion equations, now constitute the backbone in most commercial production codes, such as SIMULATE-3 [34], used by the nuclear power industry. These nodal methods are far superior to alternate finite difference or control volume approaches for the neutron diffusion equations. Furthermore, the nodal methods have a general applicability that can be utilized by other fields as well. In subsequent applications, the NIM has been developed to solve the CDE [12,26,27,30]. When compared with other schemes, such as LECUSSO [18,19] or the Crank–Nicholson four point upwinding scheme, the NIM for the CDE is found to be more efficient [27,30].

Although the NIM offers accurate results on coarse meshes, the transverse integration step limits the method to problems with domains of regular geometries (i.e., those formed by the union of rectangles). Nodal methods have been developed for specific non-rectangular geometries—such as cylindrical [3,21,24] or hexagonal [15]. However, only those based on the boundary fitted coordinate technique can be applied to domains of arbitrary geometry [23]. Hence, the conventional NIM developed for the CDE, though highly efficient, is only applicable to limited geometries. Application of the NIM to transport problems in irregular geometries therefore requires an extension to relax the restriction on domain shapes, without sacrificing the efficiency associated with nodal schemes.
Motivated by the idea proposed in the context of the steady-state heat conduction equation [32], two NIM-based hybrid numerical schemes that relax the restriction on the geometry of the computational domain while maintaining the nodal efficiency, are developed here. In these hybrid methods, the computational domain is discretized using rectangular and triangular nodes. The rectangular nodes are located in the interior of the domain and along the horizontal and vertical boundaries of the domain. The triangular nodes are used to discretize regions near any boundaries that are not aligned with the horizontal or vertical directions. In both hybrid methods, the conventional NIM is used to develop the difference scheme for the variables along the interface of adjacent rectangular nodes. A brief review of the conventional NIM is presented in Section 2.1.1. The algebraic equation for the discrete variable on the interface between a rectangular node and a triangular node is developed for the first hybrid method—the nodal-integral/finite element method (NI–FEM)—using a finite element type approach. Specifically, a trial function is written for the concentration over the triangular node in terms of the edge-averaged concentrations. Furthermore, this trial function is made to satisfy the CDE over the node in an integral sense. The discrete equation is then obtained by imposing continuity of the flux on the rectangular–triangular node interface. In the second method—the nodal-integral/finite analytic method (NI–FAM)—the algebraic equation for the interface between the two types of nodes is developed using a finite analytic approach [8–10,33]. The finite analytic method is similar to the NIM in that it reduces the governing partial differential equation(s) into a set of ordinary differential equations. However, instead of using a transverse-integration step, the partial differential equation(s) in the finite analytic method is reduced to ordinary differential equations by introducing certain assumptions and splitting the original problem into sub-problems, which can be solved analytically. These analytical solutions are then used to calculate the flux along the interface between the two types of nodes, from which the discrete equations are obtained. Exploiting the fact that the derivation of the NI–FAM is relatively simpler than the derivation of the NI–FEM, the former method is extended to solve the more general time-dependent, two-dimensional, CDE.

The remainder of this paper is organized into the following sections. Section 2 presents the formal development of the two hybrid methods for the steady-state, CDE, and the derivation of the hybrid NI–FAM for the more general time-dependent, CDE. Furthermore, this section also includes a brief review of the NIM for regular geometries. In Section 3, numerical results for both steady-state and time-dependent problems are presented and discussed. The paper is then concluded with a short summary and discussion in Section 4.

2. Formalism

2.1. Steady-state convection–diffusion equation

The steady-state CDE is

$$D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - u(x,y) \frac{\partial C}{\partial x} - v(x,y) \frac{\partial C}{\partial y} = Q(x,y),$$

where $C$ is the concentration (or temperature), $D$ is the diffusion coefficient, $u$ and $v$ are the velocities in the $x$ and $y$ directions respectively, and $Q$ is the source/sink term. The discretization of
an arbitrarily shaped computational domain, shown schematically in Fig. 1(a), is carried out for both methods by dividing it into rectangular and triangular nodes. The regions in the interior of the domain and along the horizontal and vertical boundaries are discretized using rectangular nodes, while the regions adjacent to the non-horizontal and non-vertical boundaries are discretized using triangular nodes. Only right triangular nodes are used such that the hypotenuse of each node coincides with the boundary. Schematic diagrams of the triangular and rectangular nodes with half-width and half-height of $a$ and $b$ respectively, associated discrete variables, and local coordinate system are shown in Fig. 1(b). Moreover, the discrete variables associated with the NIM and the hybrid methods are the transverse-integrated quantities along node edges (surfaces). These discrete variables will be discussed in more detail shortly.

The conventional NIM is used to calculate the discrete variables on the interfaces between adjacent rectangular nodes. A comprehensive development of the NIM for regular geometries—domains that are formed from the union of rectangular nodes—can be found in [12,26,27,31]. A brief summary of the NIM for regular geometries is outlined below.

### 2.1.1. Brief review of the NIM for the CDE in regular geometries

The two-dimensional spatial domain is first discretized into a set of $m \times n$ rectangular nodes. Each node, identified by the index $(i,j)$, is of size $2a_{i,j} \times 2b_{i,j}$. A local coordinate system
\(-a_{i,j} < x < a_{i,j}, -b_{i,j} < y < b_{i,j}\) with the origin at the center is defined for each node. Furthermore, a constant velocity in the \(x\) direction, \(\bar{u}_{i,j}^{x}\), and a constant velocity in the \(y\) direction, \(\bar{v}_{i,j}^{y}\), is assigned to each node by averaging the respective space-dependent velocity over the node. The CDE is transverse-integrated locally (i.e., over the node) in the \(x\) direction by operating in Eq. (1) with \((1/2a_{i,j}) \int_{-a_{i,j}}^{a_{i,j}} dx\), and then the procedure is repeated in the \(y\) direction by operating on the original CDE (Eq. (1)) with \((1/2b_{i,j}) \int_{-b_{i,j}}^{b_{i,j}} dy\). Thus, the transverse integration step leads to two, second order ordinary differential equations,

\[
D \frac{d^2 \tilde{C}_{i,j}^\xi(\eta)}{d\eta^2} - \mu_{i,j} \frac{d \tilde{C}_{i,j}^\xi(\eta)}{d\eta} = \tilde{S}_{i,j}^\xi(\eta) \equiv \frac{1}{2\lambda} \int_{-\lambda_{i,j}}^{\lambda_{i,j}} \left( Q - D \frac{\partial^2 C}{\partial \xi^2} + \sigma_{i,j} \frac{\partial C}{\partial \xi} \right) d\xi
\]  

(2)

for the transverse integrated variables, \(\tilde{C}_{i,j}^\xi(\eta)\), where \(\xi = x, y; \eta = y, x; \mu = u, v; \sigma = v, u; \lambda = a, b\). The right-hand side of Eq. (2) is often called the \textit{pseudo-source} term. Moreover, the use of the node-averaged velocities in the convection term is a second order approximation, which is consistent with the overall accuracy of the second order NIM [27]. Formally, the \textit{transverse-integrated} (or \textit{surface-averaged} or \textit{edge-averaged}) functions are defined as

\[
\tilde{C}_{i,j}^\eta(x) \equiv \frac{1}{2b_{i,j}} \int_{-b_{i,j}}^{b_{i,j}} C(x,y) dy;
\]

(3)

\[
\tilde{C}_{i,j}^\xi(y) \equiv \frac{1}{2a_{i,j}} \int_{-a_{i,j}}^{a_{i,j}} C(x,y) dx.
\]

(4)

The surface-averaged functions represent, respectively, the \(x\)-dependent concentration averaged locally over the node in the \(y\) direction and the \(y\)-dependent concentration averaged locally over the node in the \(x\) direction.

To solve the ordinary differential equations, the unknown inhomogeneous term on the right-hand side of Eq. (2), \(\tilde{S}_{i,j}^\xi(\eta)\), is expanded in Legendre polynomials and truncated at the zeroth order. This effectively replaces the pseudo-source term, \(\tilde{S}_{i,j}^\xi(\eta)\), with the constant, \(\tilde{S}_{i,j}^{0\xi}\). (In the development of Elnawawy et al. [12], higher order terms are retained, which leads to higher order numerical schemes.) Eq. (2) is then solved analytically for \(\tilde{C}_{i,j}^\xi(\eta)\) locally over the node \((i,j)\) using boundary conditions at \(\eta = \pm \gamma\), where \(\gamma = \alpha, \beta\). For \(\xi = y\) and \(\eta = x\), the boundary conditions are defined using the transverse-integrated (or surface-averaged or edge-averaged) variables,

\[
\tilde{C}_{i,j}^\eta(x = -a_{i,j}) = \tilde{C}_{i-1,j}^\eta,
\]

(5a)

\[
\tilde{C}_{i,j}^\eta(x = a_{i,j}) = \tilde{C}_{i,j}^\eta,
\]

(5b)

and the solution of Eq. (2) is

\[
\tilde{C}_{i,j}^\eta(x) = \left( e^{(2Pe_{x,i,j})} - e^{(Pe_{x,i,j} + (\bar{u}_{i,j}^{x}/D)x)} \right) \tilde{C}_{i-1,j}^\eta + \left( e^{(Pe_{x,i,j} + (\bar{u}_{i,j}^{x}/D)x)} \right) \tilde{C}_{i,j}^\eta
\]

\[
- \frac{a_{i,j}}{\bar{u}_{i,j}^{x}(e^{(2Pe_{x,i,j})} - 1)} \left( 1 + e^{(2Pe_{x,i,j})} - 2e^{(Pe_{x,i,j} + (\bar{u}_{i,j}^{x}/D)x)} + \frac{xe^{(2Pe_{x,i,j})}}{a_{i,j}} - x \right) \tilde{S}_{i,j}^{0\eta}
\]

(6)

where \(Pe_{x,i,j} \equiv \bar{u}_{i,j}^{x}a_{i,j}/D\). The solution for \((\xi, \eta) = (x,y)\) is obtained in a similar manner.
The numerical schemes are then developed by equating the edge-averaged fluxes on the interface between two nodes. For \((\xi, \eta) = (y, x)\), and the adjacent nodes, \((i, j)\) and \((i + 1, j)\), this conservation condition is given by

\[
D \frac{d\bar{C}^y_{ij}}{dx} \bigg|_{x=a_{ij}} = D \frac{d\bar{C}^y_{i+1,j}}{dx} \bigg|_{x=-a_{i+1,j}}.
\]

(7)

A similar equation is then obtained for \((\xi, \eta) = (x, y)\), by equating fluxes in the \(y\) direction at the interface between nodes \((i, j)\) and \((i, j + 1)\). These two equations are written in terms of the unknown (constant) pseudo-source terms, \(S^0_y, S^0_x\) and the unknown surface-averaged concentrations, \(\bar{C}^x_{i,j-1}, \bar{C}^x_{i,j}, \bar{C}^x_{i,j+1}, \bar{C}^x_{i,j+2}\). In the NIM, the discrete unknowns to be solved are these surface-averaged concentrations. Specifically, for the rectangular node, \((i, j)\), the associated discrete unknowns are \(\bar{C}^x_{i,j} \equiv \bar{C}^x_{i,j} (x = a_{ij})\), which is the surface-averaged concentration along the right surface of the node, and \(\bar{C}^x_{i,j} \equiv \bar{C}^x_{i,j} (x = b_{ij})\), which is the surface-averaged concentration along the top surface of the node. (The surface-averaged concentrations, \(\bar{C}^x_{i,j-1,} \bar{C}^x_{i,j+1}\), are associated with the nodes \((i - 1, j)\) and \((i, j - 1)\), respectively.) Consequently, two more equations are needed per node to close the set of equations. These are obtained by imposing two constraint conditions. The first constraint condition is that the CDE must be satisfied in an integral sense over the node. Integrating the CDE locally over the node (in both the \(x\) and \(y\) directions) and invoking the definition of the pseudo-source terms leads to the following equation:

\[
\bar{S}^0_y + \bar{S}^0_x = \bar{Q}^y_{ij} \equiv \frac{1}{4a_{ij}b_{ij}} \int_{-b_{ij}}^{b_{ij}} \int_{-a_{ij}}^{a_{ij}} Q(x, y) \, dx \, dy.
\]

(8)

Eq. (8) relates the node-averaged source term, \(\bar{Q}^y_{ij}\), to the two unknown (constant) pseudo-source terms. The second constraint condition ensures that each node has only one unique node-averaged concentration. That is,

\[
\bar{C}^x_{ij} \equiv \frac{1}{2a_{ij}} \int_{-a_{ij}}^{a_{ij}} \bar{C}^x_{ij}(x) \, dx = \bar{C}^x_{ij} \equiv \frac{1}{2b_{ij}} \int_{-b_{ij}}^{b_{ij}} \bar{C}^x_{ij}(y) \, dy.
\]

(9)

The two constraint conditions complete the set of equations needed to develop the numerical scheme. In practice, to obtain the difference relations in terms of the discrete unknowns only, the unknown pseudo-source terms—\(S^0_x\) and \(S^0_y\)—are eliminated algebraically in favor of the edge-averaged concentrations. This will yield the final form of the difference relations (not shown here) to solve for the discrete unknowns, \(\bar{C}^x_{ij}\) and \(\bar{C}^y_{ij}\).

The analytical solutions of the transverse-integrated differential equations lead to coefficients in the difference scheme that contain exponential terms. The incorporation of these transcendental functions allows for accurate local reconstruction of the concentration within the nodes. Furthermore, the arguments of the exponential terms are dependent on the node Peclet number. Consequently, the NIM for the CDE is characterized by “inherent upwinding”, in which the node surfaces in the upwind direction are automatically weighted more than the other node surfaces. Applications to the CDE clearly demonstrate the efficiency of the NIM, producing results of accuracy comparable to conventional numerical methods at lower CPU times [27].
In the NIM-based hybrid methods, the local concentration within the triangular nodes is formulated using the same transverse-integrated variables employed in the NIM for rectangular nodes. This maintains consistency when satisfying continuity and conservation conditions on rectangular–triangular node interfaces. The first hybrid method—the NI–FEM—is developed in Section 2.1.2. The hybrid NI–FAM is developed in Section 2.1.3.

2.1.2. Hybrid nodal-integral/finite element method

In this hybrid method, a finite element type approach is developed for the triangular nodes. The trial functions for the triangular nodes are chosen to capture the characteristics of the CDE [29] and to retain the inherent upwinding that results when applying the conventional NIM to the rectangular nodes [27]. Taking advantage of the known transverse-integrated node interior concentration variation in a rectangular node, the trial function for the triangular node in the local $x$–$y$ coordinate system is written as

$$C(x,y) = \psi_0 + \left\{ y \exp \left( \frac{\bar{u}^{xy}}{D} (a + x) \right) \right\} \psi_1 + \left\{ x \exp \left( \frac{\bar{v}^{xy}}{D} (b + y) \right) \right\} \psi_2$$

$$+ \left\{ (x-a)(y+b) \left( y - \frac{b-x}{a} \right) \right\} \psi_3,$$  \hspace{1cm} (10)

where $\psi_m$, $m = 0, 1, 2, 3$ are constants, and $\bar{u}^{xy}$ and $\bar{v}^{xy}$ are, respectively, the known node-averaged $u$ and $v$ velocities. Node-averaged velocities—rather than point values—are used here since the application of the NIM to the rectangular nodes also uses node-averaged velocities in the local solution [26,27,30]. The trial function in Eq. (10) retains some of the characteristics of the exact solution of the CDE in one dimension. The exponential terms in the second and third terms of the trial function for the triangular nodes are introduced to capture variations similar to those in the rectangular nodes. Since the exponential terms, $\exp \left( (\bar{u}^{xy}/D)(a + x) \right)$ and $\exp \left( (\bar{v}^{xy}/D)(b + y) \right)$, are solutions of the one-dimensional homogeneous CDE, these functions, by themselves, lead to a set of linearly dependent equations when $\psi_m$ ($m = 0, 1, 2, 3$) are solved in terms of the transverse-integrated discrete variables. Hence, the two exponential terms are multiplied by the independent variables, $y$ and $x$, respectively. The fourth term is zero on the boundary of the triangle, and is included to satisfy the CDE over the node in an integral sense. Note that as $\bar{u}^{xy}$ and $\bar{v}^{xy}$ tend to zero, this trial function reduces to the one used for the heat conduction equation [32].

The desired discrete variables for the triangular node, as shown in Fig. 1(b), are the surface-averaged values, $\bar{C}^x, \bar{C}^y,$ and $\bar{C}^h$ (the subscripts, $i, j$, have been omitted for convenience). The quantity, $\bar{C}^h$, is the concentration averaged along the hypotenuse of the triangular node. Similarly, $\bar{C}^x$ and $\bar{C}^y$ represent the averages over the faces parallel to the $x$ and $y$ directions, respectively. These are introduced into the trial function by requiring that the trial function must yield these edge-averaged values when integrated along each of the three edges. Hence,

$$\bar{C}^x \equiv \frac{1}{2a} \int_{-a}^{a} C(x, y = -b) \, dx,$$  \hspace{1cm} (11)

$$\bar{C}^y \equiv \frac{1}{2b} \int_{-b}^{b} C(x = a, y) \, dy$$  \hspace{1cm} (12)
and
\[
\bar{C}_i^h \equiv \frac{1}{2a} \int_{-a}^{a} C \left( x, y = \frac{b}{a} x \right) \, dx. \tag{13}
\]

To satisfy the CDE over the triangular node in an integral sense, the trial function is substituted into the CDE, and integrated over the triangular node,
\[
\frac{1}{2ab} \int_{-b}^{a} \int_{-b}^{(b/a)x} \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} - \frac{\bar{u} \cdot \nabla C}{D} - \frac{\bar{v} \cdot \nabla C}{D} \right) \, dy \, dx \\
= \frac{\bar{Q}^y}{D} \equiv \frac{1}{2abD} \int_{-a}^{a} \int_{-b}^{(b/a)x} Q(x, y) \, dy \, dx \tag{14}
\]
yielding the last of the four equations necessary to solve for \( \psi_m, m = 0, 1, 2, 3 \). Using Eqs. (11)–(14) to eliminate the coefficients, \( \psi_m \), the trial function is rewritten in terms of the surface-averaged values and the node-averaged source term,
\[
C(x, y) = f(x, y; \bar{C}^x, \bar{C}^y, \bar{C}_i^h, \bar{Q}^y). \tag{15}
\]

With the trial function written in terms of the surface-averaged concentrations, the difference scheme for the discrete variable on the interface between the two types of nodes is developed by satisfying the continuity and conservation conditions (\( C^0 \) and \( C^1 \)). In Fig. 2, the triangular node \((i, j)\) and the rectangular node \((i + 1, j)\) adjacent to it are shown. The surface-averaged concentration on the common edge shared by the triangular node, \((i, j)\), and the rectangular node on its right, \((i + 1, j)\), is \( \bar{C}_{ij}^y \). That is, the surface-averaged value on the right edge of the triangular node is equal to the surface-averaged value on the left edge of the rectangular node. Continuity of the flux on the common interface is then imposed by equating the edge-averaged flux from the right surface of the triangular node to the edge-averaged flux from the left surface of the rectangular node, \((i + 1, j)\). Hence, the trial function for the triangular node is averaged over the \( y \) direction,
differentiated with respect to $x$, evaluated at the right edge ($x = a_{i,j}$), and multiplied by $D$, to obtain

$$
D \frac{\partial \bar{C}^v_{i,j}}{\partial x} \bigg|_{x=a_{i,j}} = D \frac{\partial}{\partial x} \left( \frac{1}{2b_{i,j}} \int_{-b_{i,j}}^{b_{i,j}} C_{i,j}(x,y) \, dy \right) \bigg|_{x=a_{i,j}}.
$$

(16)

For the rectangular node, $(i+1,j)$, the corresponding $y$-averaged solution is given by $\bar{C}^v_{i+1,j}(x)$. The transverse-integrated variable, $\bar{C}^v_{i+1,j}(x)$, is given by Eq. (6) with $i$ replaced by $i + 1$. Differentiating $\bar{C}^v_{i+1,j}(x)$ with respect to $x$, evaluating it at $x = -a_{i+1,j}$, multiplying it by $D$ and equating it to the expression in Eq. (16) yields the difference equation for $\bar{C}^v_{i,j}$, which is of the form

$$
D \frac{\partial \bar{C}^v_{i,j}}{\partial x} \bigg|_{x=a_{i,j}} - D \frac{\partial \bar{C}^v_{i+1,j}}{\partial x} \bigg|_{x=-a_{i+1,j}} =
$$

$$(T^{(1)}_{i,j}) \bar{C}^v_{i-1,j} + (T^{(2)}_{i,j}) \bar{C}^v_{i,j} + (T^{(3)}_{i,j}) \bar{C}^v_{i+1,j} + (T^{(4)}_{i,j}) \bar{C}^x_{i,j} + (T^{(5)}_{i,j}) \bar{C}^v_{i,j-1} + (T^{(6)}_{i,j}) \bar{C}^x_{i,j+1} + (T^{(7)}_{i,j}) \bar{C}^x_{i+1,j} + (T^{(8)}_{i,j}) \bar{Q}^v_{i,j} + (T^{(9)}_{i,j}) \bar{Q}^v_{i+1,j} + (T^{(10)}_{i,j}) \bar{Q}^h_{i,j} = 0.
$$

(17)

The coefficients, $T^{(k)}_{i,j}$ ($k = 1, 2, 3, \ldots, 10$), are constants that depend upon node dimensions and node-averaged velocities. The expressions for these coefficients are given in Appendix A. In the case of the steady-state CDE, these coefficients are constant and need to be evaluated only once for each node. Furthermore, the difference scheme for the discrete equation $\bar{C}^v_{i,j}$, given by Eq. (17), is determined by the concentration distribution over the triangular node (which depends upon the surface-averaged values, $\bar{C}^x_{i,j-1}$, $\bar{C}^v_{i,j}$, $\bar{C}^h_{i,j}$, and the node-averaged source term, $\bar{Q}^v_{i,j}$) and by the concentration distribution over the rectangular node, $(i + 1,j)$, (which depends upon the surface-averaged values, $\bar{C}^x_{i+1,j}$, $\bar{C}^v_{i+1,j}$, $\bar{C}^h_{i+1,j-1}$, $\bar{C}^v_{i+1,j}$, and the node-averaged source term, $\bar{Q}^v_{i+1,j}$). The procedure outlined above is repeated in the $y$ direction and a difference equation is developed for $\bar{C}^x_{i,j-1}$ by equating the $x$-averaged flux on the interface between the triangular node, $(i,j)$, and the rectangular node, $(i,j-1)$.

The formalism developed above corresponds only to one type of triangular node. In practice, there will be four types of triangular nodes necessary to discretize any arbitrary shape in two dimensions. The three remaining types of triangular nodes are shown in Fig. 3(a). The hybrid scheme for the remaining triangular nodes is developed in the same manner as the derivation outlined here.

In some cases, discretization may necessitate the use of triangular nodes with common interfaces. An example of two such nodes is shown in Fig. 3(b). Difference equations for the discrete variable on the interface between two triangular nodes can also be developed following the general procedure outlined above. Moreover, the development above is carried out for the case of Dirichlet boundary conditions, in which the surface-averaged values along the hypotenuse of the triangular nodes, $\bar{C}^h_{i,j}$, are known. The hybrid method can be extended to the case of Neumann and Robin boundary conditions for $C(x,y)$. This completes the formal development of the hybrid NI–FEM.
2.1.3. Hybrid nodal-integral/finite analytic method

Similar to the NI–FEM, the discrete equations in the NI–FAM for the interface between adjacent rectangular nodes are developed using the conventional NIM, as outlined in Section 2.1.1. For the interface between a triangular node and a rectangular node, an approximate solution of the CDE is first developed for the triangular node in an ad hoc manner using the local analytic solutions to the one-dimensional CDEs in the $x$ and $y$ directions via the finite analytic approach [8–10,33]. The equations for the discrete variables are then derived by imposing continuity of the flux on the interface. The finite analytic approach developed below corresponds to the triangular node shown in Fig. 1(b). The difference relations for the other three types of triangular nodes are derived in the same manner as the one presented below.

The concentration over the triangular node, $C(x,y)$, is first approximated as the sum of two unknown functions and a constant

$$C(x,y) \cong C_x(x) + C_y(y) + C_0.$$ 

This approximation is similar to the one introduced in the finite analytic method of Chen et al. [10] and is based on the principle of superposition for linear differential equations. Furthermore, this approximation is expected to deteriorate for distributions with cross-terms such as $xy$, $x^2y$, $xy^2$, etc. Anticipating that the finite analytic approach for the triangular node will be coupled with the NIM for the rectangular nodes, the functions, $C_x(x)$ and $C_y(y)$, are approximations to single variable transverse-averaged concentrations in the triangular node. These functions respectively correspond to the transverse-integrated functions, $\bar{C}^x(x)$ and $\bar{C}^y(y)$, of a rectangular node. As will be shown, the finite analytic approach of the triangular node is developed in terms of the transverse-integrated variables so that the finite analytic approach of the triangular node can be coupled with the nodal approach of the adjacent rectangular node.
The source term, \( Q(x, y) \), is also approximated as the sum of two unknown functions, which are referred to as sub-sources,
\[
Q(x, y) \cong R(x) + S(y).
\]

The two approximations are then substituted into the CDE, and the partial differential equation is split into two ordinary differential equations with their respective boundary conditions,
\[
\begin{align*}
D \frac{d^2 C_x}{dx^2} - \bar{u}^{xy} \frac{dC_x}{dx} &= R(x), \\
C_x(x = 0) &= \bar{C}^b, \\
C_x(x = a) &= \bar{C}^y
\end{align*}
\]
and
\[
\begin{align*}
D \frac{d^2 C_y}{dy^2} - \bar{v}^{xy} \frac{dC_y}{dy} &= S(y), \\
C_y(y = 0) &= \bar{C}^b, \\
C_y(y = -b) &= \bar{C}^x.
\end{align*}
\]

Since the single variable functions of the finite analytic approximations correspond to the transverse-integrated functions of the NIM, it is consistent to use transverse-integrated variables in the boundary conditions at \( x = a, y = -b \), and at \( x = 0 \) and at \( y = 0 \) \[35\]. This facilitates the coupling of the finite analytic approach of the triangular node with the nodal approach of the adjacent rectangular node. Furthermore, the velocities in the convection term have been approximated by the node-averaged velocities, \( \bar{u}^{xy} \) and \( \bar{v}^{xy} \). As will be shown, the functions, \( C_x(x) \) and \( C_y(y) \), are unknowns that are solved explicitly, while \( R(x) \) and \( S(y) \) are unknown functions that are carried through the derivation, but not explicitly solved.

The development of the difference scheme for the NI–FAM now proceeds in a manner similar to the development of the NIM. First, Eqs. (20a)–(21c) are solved locally over a node. The unknown constants in the resulting analytical solutions are then eliminated in favor of the edge-averaged concentration of the nodes by imposing the boundary conditions and physical constraints. Satisfying the continuity of transverse-averaged concentration and the flux on the interface between the triangular–rectangular nodes then yields the difference scheme.

To solve the ODEs, Eqs. (20a)–(21c), the inhomogeneous source terms, \( R(x) \) and \( S(y) \), are expanded in Legendre polynomials, and truncated at the zeroth order. This effectively replaces the sub-sources by the unknown constants, \( R_0 \) and \( S_0 \). (The same expansion and truncation procedure is also performed in the NIM.) The ordinary differential equations are then solved. The solutions of Eqs. (20a)–(21c) are
\[
C_x(x) = \left\{ \frac{e^{(\bar{u}^{xy}x/D)} - 1}{e^{\bar{u}^{xy}x} - 1} \right\} \bar{C}^y + \left\{ \frac{e^{\bar{u}^{xy}x} - e^{(\bar{u}^{xy}x/D)}}{e^{\bar{u}^{xy}x} - 1} \right\} \bar{C}^b + \left\{ \frac{a \left(e^{(\bar{u}^{xy}x/D)} - 1\right)}{\bar{u}^{xy}(e^{\bar{u}^{xy}x} - 1) - \bar{u}^{xy}} \right\} R_0,
\]
\[
C_y(y) = \left\{ \frac{e^{(\bar{v}^{xy}y/D)} - 1}{e^{\bar{v}^{xy}y} - 1} \right\} \bar{C}^x + \left\{ \frac{e^{\bar{v}^{xy}y} - e^{(\bar{v}^{xy}y/D)}}{e^{\bar{v}^{xy}y} - 1} \right\} \bar{C}^b + \left\{ \frac{a \left(e^{(\bar{v}^{xy}y/D)} - 1\right)}{\bar{v}^{xy}(e^{\bar{v}^{xy}y} - 1) - \bar{v}^{xy}} \right\} S_0.
\]
\[ C_y(y) = \left\{ \frac{e^{Pe_y} - e^{(Pe_y+(\psi^y/D))}}{e^{Pe_y} - 1} \right\} C_x^a + \left\{ \frac{e^{(Pe_y+(\psi^y/D))} - 1}{e^{Pe_y} - 1} \right\} C_y^b + \left\{ \frac{b \left( e^{(Pe_y+(\psi^y/D))} - e^{Pe_y} \right) - y / \psi^y}{ \psi^y (e^{Pe_y} - 1) } \right\} S_0, \]

where \( Pe_x = \bar{\psi}^x a / D \) and \( Pe_y = \bar{\psi}^y b / D \). Thus, the analytical solutions for \( C_x(x) \) and \( C_y(y) \) are in terms of the surface-averaged values, \( \bar{C}_x \), \( \bar{C}_y \), and \( \bar{C}_h \), and the unknown constants, \( R_0 \) and \( S_0 \). The finite analytic approach of the triangular node can now be coupled to the NIM for the adjacent rectangular node to develop the hybrid difference scheme. As in the previous hybrid scheme (NI-FEM), continuity of the flux over the common interface of the two types of nodes, shown in Fig. 2, is satisfied by equating the flux from the right surface of the triangular node with the flux from the left surface of the rectangular node. For the triangular node, differentiation of \( C_{i,j}(x,y) \) with respect to \( x \) is equivalent to differentiation of \( C_{i,j}(x) \). The flux for the rectangular node is obtained by differentiating the \( x \)-dependent concentration averaged in the \( y \) direction for the node \((i + 1, j)\), \( \bar{C}_{i+1,j}^y(x) \), and multiplying it by \( D \). Equating these fluxes yields the difference relation for \( \bar{C}_{i,j}^x \),

\[ D \frac{\partial C_{x,i,j}}{\partial x} \bigg|_{x=a_{i,j}} - D \frac{\partial C_{x,i+1,j}}{\partial x} \bigg|_{x=-a_{i+1,j}} = (\hat{F}_{x,j}^{(1)}) \bar{C}_{i,j}^h + (\hat{F}_{x,j}^{(2)}) \bar{C}_{i,j}^y + (\hat{F}_{x,j}^{(3)}) R_{0,i,j} + (\hat{F}_{x,j}^{(4)}) \bar{C}_{i+1,j}^x, \]

where the coefficients, \( \hat{F}_{x,j}^{(m)} (m = 1, 2, 3, \ldots, 7) \), are constants that depend upon the node dimensions, and node-averaged velocities. The difference scheme for the \( y \) direction can be obtained in a similar manner by equating the appropriate derivatives,

\[ D \frac{\partial C_{y,i,j}}{\partial y} \bigg|_{y=-b_{i,j}} = D \frac{\partial C_{x,i,j-1}}{\partial y} \bigg|_{y=b_{i,j-1}}. \]

The difference schemes for the \( x \) direction and \( y \) direction respectively contain the unknowns, \( R_0 \) and \( S_0 \). Hence, two constraint conditions are needed to eliminate these two unknowns. The first constraint is obtained by substituting the truncated expansions for \( R(x) \) and \( S(y) \) into Eq. (19), and averaging the subsequent expression over the triangular node,

\[ (R_0 + S_0) = Q^y \equiv \frac{1}{2ab} \int_{-a}^{a} \int_{-b}^{b} Q(x, y) \, dy \, dx. \]

This condition ensures that the sum of the two constant sub-sources is equal to the node-averaged source term. Motivated by a similar step in the development of the NIM, the second constraint is obtained by requiring that both \( C_x(x) \) and \( C_y(y) \) yield the same node-averaged concentration when integrated in the \( x \) and the \( y \) direction, respectively. That is,

\[ \bar{C}_x^y = \frac{1}{a} \int_{0}^{a} C_x(x) \, dx = \frac{1}{b} \int_{-b}^{0} C_y(y) \, dy. \]
Using Eqs. (26) and (27), the difference scheme given by Eq. (24) can now be recast in terms of
the discrete unknowns (transverse-integrated concentrations) and the known node-averaged source
terms
\[
\begin{align*}
D \frac{\delta C_{x,i,j}}{\delta x} \bigg|_{x=a_{i,j}} - D \frac{\delta C_{x,i+1,j}}{\delta x} \bigg|_{x=a_{i+1,j}} \\
= (F_{i,j}^{(1)}) \bar{C}_{i-1,j} + (F_{i,j}^{(2)}) \bar{C}_{i,j} + (F_{i,j}^{(3)}) \bar{C}_{i+1,j} + (F_{i,j}^{(4)}) \bar{C}_{i,j} + (F_{i,j}^{(5)}) \bar{C}_{i,j-1} + (F_{i,j}^{(6)}) \bar{C}_{i+1,j} \\
+ (F_{i,j}^{(7)}) \bar{C}_{i+1,j-1} + (F_{i,j}^{(8)}) \bar{Q}_{x,i,j} + (F_{i,j}^{(9)}) \bar{Q}_{y,i+1,j} + (F_{i,j}^{(10)}) \bar{C}_{i,j} = 0, 
\end{align*}
\]
where the coefficients \( F_{i,j}^{(m)} \) (\( m = 1, 2, 3, \ldots, 10 \)) are constants that depend upon node
dimensions and node-averaged velocities. The expressions for the coefficients, \( F_{i,j}^{(m)} \), are given in
Appendix B. The corresponding difference scheme for the surface-averaged variable \( \bar{C}_{i,j-1} \), shown
in Fig. 2, is developed by equating the flux on the interface between the triangular node \((i, j)\) and
the rectangular node \((i, j - 1)\). This completes the derivation of the hybrid NI–FAM for
the steady-state CDE.

2.2. Formalism for the time-dependent convection–diffusion equation

Numerical results, presented later in Section 3, show that the NI–FEM for the steady-state
CDE is more accurate at very small Peclet numbers than the NI–FAM. However, on average, the
NI–FAM fares better than the NI–FEM over a wide range of Peclet numbers. Furthermore, the
development of the NI–FAM is relatively simpler than the development of the NI–FEM. Con-
sequently, only the NI–FAM has been developed for the time-dependent CDE.

The two-dimensional, time-dependent CDE is
\[
\frac{\partial C}{\partial t} + Q(x, y, t) = D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - u(x, y, t) \frac{\partial C}{\partial x} - v(x, y, t) \frac{\partial C}{\partial y},
\]
where \( C, u, v, \) and \( Q \) are now time dependent. The time axis is discretized with a constant time
interval of \( 2\sigma \). The discretization of an arbitrarily shaped, two-dimensional, spatial computational
domain proceeds by dividing the space–time domain into parallelepiped space–time nodes and
wedge-shaped, space–time nodes. The triangular node of the steady-state development becomes,
for the time-dependent problem, a wedge-shaped, space–time node. These wedge-shaped nodes
are restricted to the boundaries that are not parallel to the \( x \) or \( y \) axes. Schematic diagrams of
these parallelepiped and wedge-shaped space–time nodes with their respective discrete variables
and local coordinate systems are shown in Fig. 4(a) and (b). Before developing the NI–FAM for
the time-dependent problem, a brief overview of the conventional NIM for the two-dimensional,
time-dependent CDE is presented.

Discrete variables on the interfaces between parallelepiped nodes are determined using the
conventional NIM. Previous applications of the NIM to the time-dependent CDE have focused
either on the steady-state, two-dimensional problem [27] (also outlined in Section 2.1.1), or the
time-dependent, one-dimensional problem [30]. The cell analytical numerical method, which uses
a nodal approach for space discretization and finite difference time discretization, has also been
successfully applied to the time-dependent, two-dimensional CDE [12]. The development of the
conventional NIM for the time-dependent, two-dimensional CDE in *regular geometries* can be developed by, for example, extending the one-dimensional, time-dependent case to two dimensions. For the time-dependent CDE with three independent variables, the transverse integration step of the conventional NIM reduces the original partial differential equation into a set of three ordinary differential equations: one for each of the transverse-integrated functions, \( \bar{\mathcal{C}}^{xt}(y) \), \( \bar{\mathcal{C}}^{yt}(x) \), and \( \bar{\mathcal{C}}^{xy}(t) \). Formally, these transverse-integrated functions are defined as

\[
\bar{\mathcal{C}}^{xt}(y) \equiv \frac{1}{4a\tau} \int_{-\tau}^{\tau} \int_{-a}^{a} C(x, y, t) \, dx \, dt,
\]

(30)

\[
\bar{\mathcal{C}}^{yt}(x) \equiv \frac{1}{4b\tau} \int_{-\tau}^{\tau} \int_{-b}^{b} C(x, y, t) \, dy \, dt,
\]

(31)

\[
\bar{\mathcal{C}}^{xy}(t) \equiv \frac{1}{4ab} \int_{-b}^{b} \int_{-a}^{a} C(x, y, t) \, dx \, dy.
\]

(32)

Fig. 4. (a) Schematic diagram of the parallelepiped space–time node with its associated discrete unknowns. (b) Schematic diagram of the wedge-shaped space–time node with its associated discrete unknowns.
The right-hand sides of Eqs. (30) and (31) represent the concentration averaged locally over time and one spatial dimension, while that of Eq. (32) represents the time-dependent concentration, averaged locally over space. Applying the rest of the steps of the NIM leads to a set of three discrete equations for the three discrete variables—\( \bar{C}_{i,j,k}^\alpha \), \( \bar{C}_{i,j,k}^\beta \), and \( \bar{C}_{i,j,k}^\gamma \)—for each node \((i, j, k)\). The details are straightforward and are omitted here.

As with the steady-state formalism, the use of the surface-averaged concentrations as discrete unknowns in the NIM for the time-dependent CDE requires that the difference schemes for the interface values between parallelepiped nodes and wedge-shaped nodes be developed in terms of the same (transverse-integrated) variables [35]. In the following, a derivation of the NI–FAM (as applied to the time-dependent CDE) for the wedge-shaped node of Fig. 4(b) is presented. The development of the difference schemes for the other types of wedge-shaped nodes proceeds in a similar manner.

To develop the finite analytic scheme for the wedge-shaped nodes of the time-dependent problem, the concentration distribution is assumed to be of the form,

\[
C(x, y, t) \approx C_x(x) + C_y(y) + C_t(t) + C_0.
\]  

(33)

This approximation is similar to that made in the finite analytic method of Chen et al. [10]. The time-dependent source term over the triangular node is similarly approximated as

\[
Q(x, y, t) \approx R(x) + S(y) - T(t).
\]  

(34)

(As a matter of convenience, the sub-source term, \( T(t) \), is subtracted, rather than added, for it makes the right-hand side of Eq. (37a) positive rather than negative.) After substituting the concentration and source term approximations into Eq. (29), the CDE is split into three ordinary differential equations with their respective boundary or initial conditions,

\[
D \frac{d^2 C_x}{dx^2} - \bar{v}^{yt} \frac{dC_x}{dx} = R(x),
\]  

(35a)

\[
C_x(x = 0) = \bar{C}^{bt},
\]  

(35b)

\[
C_x(x = a) = \bar{C}^{yt},
\]  

(35c)

\[
D \frac{d^2 C_y}{dy^2} - \bar{v}^{yx} \frac{dC_y}{dy} = S(y),
\]  

(36a)

\[
C_y(y = 0) = \bar{C}^{by},
\]  

(36b)

\[
C_y(y = -b) = \bar{C}^{by},
\]  

(36c)

and

\[
\frac{dC_t}{dt} = T(t),
\]  

(37a)

\[
C_t(t = -\tau) = \bar{C}^{yx},
\]  

(37b)
where $\bar{u}_0^\text{st}$ and $\bar{v}_0^\text{st}$ are the local $u$ and $v$ velocities averaged over the space–time node. As in the steady-state case, the transverse-integrated variables are used in the boundary conditions of the above differential equations. For the wedge-shaped node of Fig. 4(b), the formal definitions of the transverse-integrated variables are

\[
\bar{C}^\text{st} \equiv \frac{1}{4at} \int_{-a}^{a} \int_{-t}^{t} C(x, y = -b, t) \, dt \, dx,
\]

\[
\bar{C}^\text{st} \equiv \frac{1}{4bt} \int_{-b}^{b} \int_{-t}^{t} C(x = a, y, t) \, dt \, dy,
\]

\[
\bar{C}^\text{ht} \equiv \frac{1}{4at} \int_{-a}^{a} \int_{-t}^{t} C\left(x, y = \frac{b}{a}, t \right) \, dt \, dx
\]

and

\[
\bar{C}^\text{vy} \equiv \frac{1}{2ab} \int_{-a}^{a} \int_{-b}^{(b/a)x} C(x, y, t = -\tau) \, dy \, dx.
\]

Following the procedure of the NI–FAM for the steady-state case, the inhomogeneous sub-source terms are expanded, truncated at the zeroth order, and the ordinary differential equations of Eqs. (35a)–(35c), (36a)–(36c), (37a), (37b) are solved locally over a node. The expansion and truncation process replaces the sub-sources, $R(x)$, $S(y)$, and $T(t)$ with the respective sub-source constants, $R_0$, $S_0$, and $T_0$. Since Eqs. (35a)–(35c), (36a)–(36c) are in forms similar to the steady-state formulations given by Eqs. (20a)–(20c), (21a)–(21c), their analytical solutions are given by Eqs. (22) and (23) with the following substitutions: $\bar{C}^x \rightarrow \bar{C}^\text{st}$, $\bar{C}^y \rightarrow \bar{C}^\text{st}$, and $\bar{C}^h \rightarrow \bar{C}^\text{ht}$. Eq. (37a) is first order and hence the analytical solution for $C_i(t)$ is linear in time,

\[
C_i(t) = \bar{C}^\text{vy} + (t + \tau)T_0.
\]

With the analytical expressions for $C_x(x)$, $C_y(y)$, and $C_i(t)$ given by Eqs. (22), (23) and (42), the finite analytic method for the wedge-shaped node can now be coupled with the NIM for the adjacent parallelepiped node to develop the hybrid scheme. In Fig. 5, the projections of the wedge-shaped node, $(i, j)$, along with its adjacent parallelepiped nodes, $(i + 1, j)$ and $(i, j - 1)$, are shown. The transverse-integrated concentration on the common edge shared by the wedge-shaped node and the parallelepiped node on its right is $\bar{C}_{i,j}^\text{st}$. Continuity requires that this surface-averaged concentration on the right edge of the wedge-shaped node be equal to the surface-averaged value on the left edge of the parallelepiped node, $(i + 1, j)$. Conservation is then satisfied by equating the flux on the right surface of the wedge-shaped node to the flux on the left surface of the rectangular node, $(i + 1, j)$. Equating the fluxes produces the difference relation for $\bar{C}_{i,j}^\text{st}$,

\[
D \frac{\partial C_{x,i,j}}{\partial x} \bigg|_{x=x_{-a}} - D \frac{\partial C_{i+1,j}^\text{st}}{\partial x} \bigg|_{x=x_{a+1}} = (\hat{G}_{i,j}^{(1)})\bar{C}_{i,j}^\text{ht} + (\hat{G}_{i,j}^{(2)})\bar{C}_{i,j}^\text{st} + (\hat{G}_{i,j}^{(3)})R_{0,i,j} + (\hat{G}_{i,j}^{(4)})\bar{C}_{i+1,j}^\text{st} + (\hat{G}_{i,j}^{(5)})\bar{C}_{i+1,j}^\text{ht} + (\hat{G}_{i,j}^{(6)})\bar{C}_{i+1,j-1}^\text{st} + (\hat{G}_{i,j}^{(7)})\bar{Q}_{i+1,j,k}^\text{st} = 0,
\]
where the coefficients, $G^{(n)}_G (n = 1, 2, 3, \ldots, 7)$, are constants that depend upon the node dimensions, the diffusion coefficient, and node-averaged velocities. Furthermore, the third subscript, $k$, which appears in certain transverse-integrated variables, refers to the current time step. Following a similar procedure in the $y$ direction, a difference relation can be obtained for the surface averaged concentration, $C^{xy}_{i,j,k}$.

Since the differential equation for $C_t(t)$ is first order, the difference scheme in the time direction is developed by simply evaluating Eq. (42) at $t = +\tau$,

$$C_t(+\tau) = \bar{C}^{xy}_{i,j,k} + (2\tau)T_{0,i,j,k} = \bar{C}^{xy}_{i,j,k},$$

(44)

where $\bar{C}^{xy}_{i,j,k} \equiv C_{t,k}(t = +\tau)$ and $\bar{C}^{xy}_{i,j,k-1} \equiv C_{t,k-1}(t = -\tau)$. Hence, Eq. (44) relates the surface-averaged concentration at the $k$th time step, $C_{i,j,k}$, to the surface-averaged concentration at the $(k-1)$st time step, $C_{i,j,k-1}$.

The difference relations for the $x$, $y$, and time directions contain the unknown sub-source constants, $R_0$, $S_0$, and $T_0$ which need to be eliminated in favor of the discrete variables, $C^{xt}$, $C^{yt}$, $C^{xy}$ and the known node-averaged source term, $\bar{Q}^{yt}$, by imposing three constraint conditions. (The node identifying subscripts, $(i,j,k)$, have been omitted.) The first constraint is obtained by substituting the truncated expansions for $R(x)$, $S(y)$, and $T(t)$ into Eq. (34) and then integrating the subsequent expression over the wedge-shaped node. This constraint ensures that the sum of the three approximated sub-source constants is equal to the node-averaged source term,

$$R_0 + S_0 - T_0 = \bar{Q}^{yt} = \frac{1}{4ab\tau} \int_{-a}^{a} \int_{-b}^{b} \int_{-\tau}^{\tau} Q(x, y, t) \, dy \, dx \, dt.$$ (45)

As with the steady-state case, the other two constraint conditions are obtained by requiring that $C_x(x)$, $C_y(y)$, and $C_t(t)$ yield the same node-averaged concentration, $\bar{C}^{yt}$, when integrated in the $x$ direction, $y$ direction and time direction, respectively. That is,
The diffusion coefficient, and node-averaged velocities. The expressions for the coefficients,

\[ C_{\text{dry}} = \frac{1}{a} \int_0^a C_x(x) \, dx = \frac{1}{2\tau} \int_{-\tau}^{\tau} C_i(t) \, dt \]  

(46)

and

\[ C_{\text{dry}} = \frac{1}{b} \int_{-b}^{0} C_y(y) \, dy = \frac{1}{2\tau} \int_{-\tau}^{\tau} C_i(t) \, dt. \]  

(47)

Using Eqs. (45)–(47), the difference scheme of Eq. (43) can be now recast only in terms of the
unknown transverse-integrated discrete variables and the known node-averaged source terms,

\[
\begin{align*}
(G_i)_{j,j}^{(1)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(2)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(3)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(4)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(5)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(6)} C_{\text{dry}}^{i,j} \\
+ (G_i)_{j,j}^{(7)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(8)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(9)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(10)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(11)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(12)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(13)} C_{\text{dry}}^{i,j} + (G_i)_{j,j}^{(14)} C_{\text{dry}}^{i,j} = 0,
\end{align*}
\]

(48)

where the coefficients, \( G_i^{(p)} \) \( (p = 1, 2, \ldots , 14) \), are constants that depend upon the node dimensions, the diffusion coefficient, and node-averaged velocities. The expressions for the coefficients, \( G_i^{(p)} \), are given in Appendix C. Repeating the same procedure in the \( y \) direction leads to a discrete equation for the discrete variable, \( C_{\text{dry}}^{i,j} \). For the time direction, eliminating \( T_{0,i,j} \) in Eq. (44) leads to

\[
\begin{align*}
(H_i)_{j,j}^{(1)} C_{\text{dry}}^{i,j} + (H_i)_{j,j}^{(2)} C_{\text{dry}}^{i,j} + (H_i)_{j,j}^{(3)} C_{\text{dry}}^{i,j} + (H_i)_{j,j}^{(4)} C_{\text{dry}}^{i,j} + (H_i)_{j,j}^{(5)} C_{\text{dry}}^{i,j} \\
+ (H_i)_{j,j}^{(6)} C_{\text{dry}}^{i,j} + (H_i)_{j,j}^{(7)} C_{\text{dry}}^{i,j} + (H_i)_{j,j}^{(8)} C_{\text{dry}}^{i,j} = 0,
\end{align*}
\]

(49)

where \( H_i^{(q)} \) \( (q = 1, 2, 3, \ldots , 8) \) are constants that depend upon the node dimension, the diffusion coefficient, and node-averaged velocities. The expressions for the coefficients, \( H_i^{(q)} \), are given in Appendix D. Since the transverse-integrated variables, \( C_{\text{dry}}, C_{\text{dry}}, C_{\text{dry}} \), are obtained from the current time step, the difference scheme in Eq. (49) is implicit. As mentioned previously, the development here corresponds to the wedge-shaped node given in Fig. 4(b). The derivation of the difference relations for the other types of wedge-shaped nodes is similar to the development presented here. This completes the formal derivation of the hybrid NI–FAM.

2.3. Iterative solution and implementation using FORTRAN 90

A flow chart that summarizes the algorithm used by the NIM and the hybrid methods is
presented in Fig. 6. This flow chart is valid for both transient and steady-state problems. The set
of discrete equations in the NIM and the hybrid methods are solved by iteratively sweeping
through the computational domain. Specifically, the discrete variables for each node are evaluated
in a row by row fashion. A Gauss–Seidel update is performed during the sweeps and the calcula-
tion is completed when convergence, as specified by a predefined tolerance, is reached. In
time-dependent problems, this iteration procedure is carried out over the computational domain
for each time step.

The hybrid methods have been implemented using FORTRAN 90. Taking advantage of the
advanced features of FORTRAN 90, the field variables and constants associated with these
difference equations are efficiently grouped into aggregate data structures. These data structures
allow for quick and efficient handling of variables, thereby simplifying the implementation of the hybrid methods. Furthermore, to facilitate the application of the hybrid methods to a wide range of problems, the dynamic memory allocation and allocatable array capabilities of FORTRAN 90 are utilized in the implementation. Hence, certain variables are allocated (and deallocated) space on \textit{as-needed} basis during run time.

3. Numerical results and discussion

Several problems have been solved numerically using the schemes developed in the previous sections. The results of one steady-state and two time-dependent problems are presented here.
3.1. Steady-state convection–diffusion equation

A schematic diagram of the first test problem, chosen because it has an available analytic solution is shown in Fig. 7. Previously used by Faghri et al. [13] to test a control volume scheme, the objective of this problem is to calculate the temperature distribution in the flow between two parallel plates with a constant heat flux, \( q \), imposed on both plates. The flow is fully developed and laminar, with the velocity in the \( x \) direction given by

\[
u(y) = \frac{3}{2} \bar{u} \left(1 - \left(\frac{y}{h}\right)^2\right),
\]

where \( \bar{u} \) is the mean velocity in the channel and \( h \) is the channel half-height. (Unlike the previous chapter, where \( x \) and \( y \) were local to the nodes, in these sample problems, the same symbols represent global coordinates.) The exact temperature distribution in the channel is given by

\[
T(x, y) = \left(\frac{qh}{k}\right) \left\{ \left(\frac{3}{4}\right) \left(\frac{y}{h}\right)^2 \left(1 - \frac{y^2}{6h^2}\right) + \left(\frac{4}{Pe}\right) \left(\frac{x}{h}\right) \right\}.
\]

where \( q \) is the heat flux, \( k \) is the fluid thermal conductivity, \( \alpha \) is the thermal diffusivity, and the global Peclet number is defined as \( Pe = \frac{4\bar{u}h}{\alpha} \). The factor of four is retained in the definition of the Peclet number to allow comparisons with the results of Faghri et al. [13]. The two hybrid schemes developed in the previous chapter are applied to determine the temperature distribution over the irregular computational domain, \( ABCD \), also shown in Fig. 7. In the figure, point \( A \) is at \((x = 0.9090, y = -0.9090)\) and \( B \) is at \((x = 3.0277, y = 1.2123)\) with edge \( AD \) at an angle of 45° from the horizontal. Edge \( BC \) is parallel to edge \( AD \). Furthermore, computations are carried out in coordinate system \((x', y')\), shown in Fig. 7, with its origin located at point \( A \) and rotated 45° clockwise with respect to the global coordinate system \((x, y)\). Using the exact solution, Dirichlet boundary conditions are imposed on all four boundaries of the trapezoidal region, including the edge \( CD \).

The temperature distribution for different Peclet numbers is determined using the hybrid methods with \( h = 2.5 \) and \( (qh/k) = 1.0 \). Specifically, the Peclet number is varied by keeping \( \alpha = 1.0 \), while varying \( \bar{u} \), the mean velocity in the channel. Moreover, for each Peclet number, the

![Fig. 7. Schematic diagram of parallel plate channel problem and the computational domain.](image-url)
problem is solved with three different node sizes. Mesh 1, which uses a node size of \( \Delta x = 0.75 \), is the coarsest with only 22 nodes (18 rectangular and four triangular nodes). Mesh 2 with a node size of \( \Delta x = 0.375 \) has a total of 84 nodes, which consists of 76 rectangular nodes and eight triangular nodes. Finally, mesh 3, which is the finest at \( \Delta x = 0.1875 \), has a total of 186 nodes, which consists of 174 rectangular nodes and 12 triangular nodes.

For mesh 1, the numerically calculated temperature profiles along the line \( EF \), also shown in Fig. 7, are compared in Fig. 8(a) and (b) with the exact solution for Peclet numbers, \( Pe = 0.7 \) and 70.0. The agreement between the numerical and exact results for this coarse mesh is very good. For the finer meshes, the numerical results are indistinguishable from the exact results. As a more

Fig. 8. NI-FEM and NI-FAM results for mesh 1 of the steady-state parallel plate channel problem: (a) \( Pe = 0.7 \) and (b) \( Pe = 70.0 \).
quantitative comparison, and to measure the performance of the hybrid methods, the root mean square (RMS) errors of the node-averaged temperature, $T_v$, over the entire computational domain are tabulated in Table 1. The results for a new Peclet number, $Pe = 700.0$, are added to test the hybrid schemes for convection-dominated regimes.

For the three Peclet numbers tested here, the RMS errors of both the NI–FEM and the NI–FAM are reduced by a factor of approximately $\sim 2.5–3.7$ as the resolution is increased from mesh 1 ($\Delta x = 0.75$) to mesh 2 ($\Delta x = 0.375$). However, in comparing the RMS errors from mesh 2 ($\Delta x = 0.375$) to mesh 3 ($\Delta x = 0.1875$), the reduction factors decrease to approximately $\sim 2$. As an illustration of the reduction factors, Fig. 9 shows a plot of the RMS error versus node size for both methods at a Peclet number of $Pe = 0.7$. The second set of reduction factors suggests that the hybrid methods are only first order, while the first set of reduction factors suggests that the hybrid methods are higher than first order. Although a numerical scheme may be proven to be of second order, for certain resolutions or mesh sizes, the numerical scheme may exhibit less than second order behavior. This is probably the case for the two hybrid methods.

For Peclet numbers up to $Pe = 100.0$, the NI–FEM is found to be slightly better than the NI–FAM. However, for larger Peclet numbers, the NI–FEM deteriorates somewhat, but only for large node sizes, as indicated by the increase in RMS error for the coarsest mesh. This is probably the result of artificial diffusion, which tends to enhance transport in directions normal to the local flow [29]. Furthermore, the NI–FAM is very accurate over a range of Peclet numbers for the three

<table>
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<tbody>
<tr>
<td>Mesh 1 (22 nodes)</td>
<td>0.0034</td>
<td>0.0416</td>
<td>0.0033</td>
<td>0.0074</td>
<td>0.0599</td>
<td>0.0082</td>
</tr>
<tr>
<td>Mesh (84 nodes)</td>
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<td>0.0013</td>
<td>0.0027</td>
<td>0.0015</td>
<td>0.0028</td>
</tr>
<tr>
<td>Mesh 3 (186 nodes)</td>
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<td>0.0051</td>
<td>0.0007</td>
<td>0.0015</td>
<td>0.0007</td>
<td>0.0015</td>
</tr>
</tbody>
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Table 1
RMS errors for the steady-state parallel plate channel problem

Fig. 9. RMS error versus node size for both hybrid methods at $Pe = 0.7$. 
node sizes tested here, yielding RMS errors of less than 0.01 for Peclet numbers as large as $Pe = 10^{20}$.

To compare with the control volume scheme of Faghri et al. [13], the parallel-plate problem is also solved over the same domain as used by Faghri et al. This new domain has the same trapezoidal shape as the previous domain, but is slightly larger. For $Pe = 0.7$, Faghri et al. [13] reports a maximum normalized error of slightly over 1% for a mesh of 272 points. The corresponding maximum normalized error for the NI–FEM and the NI–FAM with only 39 nodes are 0.14% and 3%, respectively. At $Pe = 70.0$, Faghri et al. [13] reports a maximum normalized error of 3.7% for the 272 point mesh. The corresponding errors for the NI–FEM and NI–FAM with only 39 nodes are 1.9% and 2.2%, respectively. These results clearly show that the hybrid schemes can achieve the same or better accuracy as those of more conventional control volume type schemes with far fewer nodes (or control volumes).

### 3.2. Time-dependent convection–diffusion equation

#### 3.2.1. Temperature distribution in a parallel plate channel

As a preliminary test of the hybrid NI–FAM for time-dependent problems, the first steady-state parallel plate channel problem solved in the previous section is solved as a time-dependent problem. The temperature is allowed to evolve from an initial condition of $T(x, y, t = 0.0) = 0.0$. The NI–FAM for the time-dependent CDE yields the same results as the NI–FAM for the steady-state problem for the three meshes and three Peclet numbers used previously.

#### 3.2.2. Temperature distribution in a parallel plate channel with a source term

The second time-dependent problem is again a variation of the first parallel plate problem discussed in Section 3.1. Removing the imposed constant heat flux on the walls and introducing a space and time-dependent source term of the form

$$Q(x, y, t) = -A(c e^{-ct}) f(x, y);$$

$$f(x, y) = \left(\frac{3}{4}\right) \left(\frac{y}{h}\right)^2 \left(1 - \frac{y^2}{6h^2}\right) + \left(\frac{4}{Pe}\right) \left(\frac{x}{h}\right)$$

in the flow between the two parallel plates, the exact solution of the CDE is given by

$$T(x, y, t) = A(1 - e^{-ct}) f(x, y),$$

where $c$ is a positive constant and $A$ is a normalization factor. Hence, the temperature distribution evolves from zero everywhere at time $t = 0.0$ to a steady-state solution given by Eq. (52b) (multiplied by the normalization factor) in the limit of $t \to \infty$. The computational domain for this problem is the same trapezoidal region used in the first problem of Section 3.1. The exact solution is used to impose the time-dependent Dirichlet boundary conditions. Furthermore, the flow field remains steady and is given by Eq. (50). Using $h = 2.5$, $A = 1.0$, and $c = 0.01$ the temperature evolution is calculated for three different Peclet numbers, $Pe = 0.7$, 70.0, and 700.0 on the same three meshes used in the first steady-state problem. As before, setting $\alpha = 1.0$, the Peclet number is varied by changing $\bar{u}$, the mean velocity in the channel. The choice of $c = 0.01$ leads the temperature distribution to virtually reach steady
state at a time of \( t = 1000.0 \). The temperature distributions are then calculated for \( 0.0 \leq t \leq 1000.0 \) in time steps of \( \Delta t = 1.0 \).

For mesh 1 (22 nodes), the numerically calculated node-averaged temperatures, \( T^{\text{num}} \), along the line \( EF \) are compared in Fig. 10(a)–(c) with the exact solution for the Peclet numbers, \( Pe = 0.7, 70.0, \) and 700.0. The temperature distributions shown are averaged over \( 49 < t < 50, \ 199 < t < 200, \) and \( 999 < t < 1000. \) In general, the NI–FAM performs quite well even on this coarse mesh, producing results for all three Peclet numbers that are in good agreement with the exact solution. At the lowest Peclet number of \( Pe = 0.7, \) the results obtained using the NI–FAM are nearly indistinguishable from the exact solution. At the higher Peclet numbers of \( Pe = 70.0 \) and 700.0, however, there are slight errors at the last node, which correspond to the wedge-shaped nodes. Nevertheless, the results for all Peclet numbers are very accurate considering the coarseness of the mesh.

Fig. 11(a) and (b) show the numerical results on mesh 2 (84 nodes) for the Peclet numbers, \( Pe = 0.7 \) and 700.0. Once again, the results of the hybrid method are very accurate, with very
small differences when compared with the exact solution. Fig. 12 shows the results on mesh 3 (186 nodes) for a Peclet number of $Pe = 700.0$. The results for mesh 3, which is the most refined of the three meshes, are virtually identical to the exact solution. The results in Figs. 10–12 show that the error at the last node continues to decrease with decreasing mesh size. This indicates that the decrease in accuracy due to the wedge-shaped node can be compensated with a small degree of mesh refinement.

3.2.3. Advection of a Gaussian concentration hill in a rotating flow field

In this problem, solute with a Gaussian distribution is advected in a rotating flow field. This almost pure advection problem (high Peclet number) is simulated to test the ability of the NI–FAM to capture the location and magnitude of a moving concentration peak. Several variations
of this problem have been used to test conservative numerical schemes for advection problems [5,25]. Furthermore, variations of this problem also serve as difficult benchmark problems to test the performance of numerical schemes for the CDE in the advection limit [7,11].

The computational domain for this problem is the circular region centered at (2.0, 2.0) with a radius of 2.0 spatial units, shown in Fig. 13. The rotating flow field is given by

$$\vec{V} = 2\pi \left( \frac{2 - y}{x - 2} \right).$$

(54)

with the initial concentration distribution, given by

$$C(x, y, t = 0) = \exp \left( - \frac{(x - x_0)^2}{2\sigma^2} - \frac{(y - y_0)^2}{2\sigma^2} \right).$$

(55)

The center of the hump, with a standard deviation of $\sigma_x = \sigma_y = 0.15$, is initially placed at $(x_0 = 2.86, y_0 = 2.86)$. Furthermore, the initial concentration field is evaluated only within $4\sigma$ of the center of the hump, while the concentration outside of this circular region is initially set to zero. Moreover, the flow field is configured such that the center of the hump, which is on the diagonal line $CA$ at $t = 0.0$ will advect one complete rotation in one time unit. A (dashed) streamline in Fig. 13 denotes the path of the center of the hump.

Using a uniform node size of $\Delta x = \Delta y$ and a uniform time step of $\Delta t = 2\tau$ the space–time computational domain is discretized with wedge-shaped nodes and parallelepiped nodes. As described in the formalism, the wedge-shaped nodes are restricted to the boundaries of the circular domain. The problem is solved over the time interval, $0.0 \leq t \leq 1.0$. To simulate nearly pure advection, a diffusion coefficient of $D = 10^{-5}$ is used. The node Peclet number is defined as $Pe_{node} = U_{node} \Delta x / D$, where $U_{node}$ is the node-averaged speed. Hence, minimal diffusion and minimal spreading of the hump are expected over the time interval since the Peclet number is large.
The concentration distribution is first evaluated for the uniform node size of $\Delta x = \Delta y = 0.04$ and $\Delta t = 0.005$. The maximum nodal Peclet number for this problem is $Pe_{\text{node}} \sim 32,000$. The plot in Fig. 14 shows the spatially averaged concentration profile, $\bar{C}^y$, as a function of the node number along the lines $AB$ (at $t = 0.0, 1.0$), $AC$ (at $t = 0.25$), $AD$ (at $t = 0.5$), and $AE$ (at $t = 0.75$). The numerical scheme captures the location of the peak very faithfully over the entire simulation period. The magnitude of the peak is also calculated quite accurately for the first 0.25

Fig. 13. Schematic diagram of the Gaussian concentration hill advected in a rotating flow field.

Fig. 14. NI–FAM results for advection of a Gaussian concentration hill with uniform mesh of $\Delta x = \Delta y = 0.04$. 

time units. However for $t > 0.25$, the accuracy of the hybrid method in determining the magnitude of the peak decreases such that by $t = 1.00$ the peak has dropped to a value of 0.94445 from its original value of 0.99410. Although the magnitude of the peak does decrease, as shown in the results, there is very little spreading during the rotation. The simulation is repeated for a second mesh, which has a uniform node size of $\Delta x = \Delta y = 0.02$ and a time step of $\Delta t = 0.0025$. The results for the second mesh are shown in Fig. 15. For this finer mesh, the NI–FAM performs very well, accurately capturing the location and magnitude of the peak over the entire time interval with essentially zero numerical diffusion.

4. Summary and conclusions

The hybrid NI–FEM and the hybrid NI–FAM have been developed to solve the steady-state CDE in arbitrary geometries. In both hybrid methods, the computational domain is discretized using rectangular nodes and triangular nodes, with the latter restricted to boundaries that are not parallel to the $x$ or $y$ axes. For the two methods, the difference schemes for the variables on the interface between adjacent rectangular nodes are developed using the conventional NIM. In the NI–FEM, a finite element type approach is combined with the nodal approach to derive the numerical scheme for the discrete variables on the interfaces between the triangular and rectangular nodes. In the NI–FAM, a finite analytic type method replaces the finite element approach of the NI–FEM. Both hybrid methods are then applied to determine the steady-state temperature distribution in a parallel plate channel with fully developed laminar flow. For Peclet numbers up to $Pe \sim 100$, both methods perform very well, and the results are in excellent agreement with the exact solution. Furthermore, both hybrid methods applied to a very coarse mesh of 39 nodes produce results with accuracy comparable to the control volume scheme of Faghri et al. [13]
applied to a mesh consisting of 272 points. Although the NI–FAM is accurate even for Peclet numbers as high as $Pe = 10^{20}$, the NI–FEM deteriorates slightly as the Peclet number is increased beyond $Pe \sim 100$, probably due to artificial diffusion.

The hybrid NI–FAM is then extended to solve the time-dependent CDE. The computational domain is discretized with parallelepiped space–time nodes and wedge-shaped space–time nodes. As before, the standard NIM is applied to the variables on the interface between adjacent parallelepiped nodes, while a hybrid nodal-integral/finite analytic approach is used to develop the numerical schemes for discrete variables on the interfaces between the two different types of nodes. The first set of problems used to test the NI–FAM for the time-dependent CDE consists of two time-dependent versions of the temperature distribution in a parallel plate channel. The numerical results are in excellent agreement with the exact solution. Moreover, steady-state results obtained from the time-dependent problem are virtually identical to the results obtained from the steady-state problem. Although the results of the hybrid method for the time-dependent problem did indicate a slight drop in accuracy for the wedge-shaped nodes, this decrease is easily compensated with a small degree of mesh refinement.

The last and much more challenging problem solved using the NI–FAM is the advection of a Gaussian concentration distribution in a high Peclet number, two-dimensional, rotating flow field in a circular domain. For a uniform node size of $\Delta x = \Delta y = 0.02$, and a time step of $\Delta t = 0.0025$, the location as well as the magnitude of the moving peak are captured very accurately over the entire simulation period, $0.0 \leq t \leq 1.0$. These benchmark problems clearly show that the NI–FEM and NI–FAM are robust and accurate numerical schemes capable of solving convection–diffusion problems in arbitrary domains for a wide range of Peclet numbers.

Acknowledgements

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Appendix A. NI–FEM difference scheme for the steady-state convection–diffusion equation

The NI–FEM difference scheme shown below for $\bar{C}^\nu_{i,j}$ (see Fig. 16) corresponds to one type of rectangular–triangular node interface. Difference schemes for the additional types of rectangular–triangular node interfaces (see Figs. 2 and 3(a)) are similar and can be easily derived following the approach presented in Section 2.1.2. The coefficients, $g$, $h$, $g_{tm}$, and $h_{tm}$, are given in Appendix E.

\begin{align*}
(T_{i,j}^{(1)}) & \bar{C}^\nu_{i-1,j} + (T_{i,j}^{(2)}) \bar{C}^\nu_{i,j} + (T_{i,j}^{(3)}) \bar{C}^\nu_{i+1,j} + (T_{i,j}^{(4)}) \bar{C}^\nu_{i,j-1} + (T_{i,j}^{(5)}) \bar{C}^\nu_{i,j+1} + (T_{i,j}^{(6)}) \bar{C}^\nu_{i,j} \\
& + (T_{i,j}^{(7)}) \bar{C}^\alpha_{i+1,j-1} + (T_{i,j}^{(8)}) \bar{Q}^{\nu}_{i,j} + (T_{i,j}^{(9)}) \bar{Q}^{\nu}_{i+1,j} + (T_{i,j}^{(10)}) \bar{Q}^h = 0,
\end{align*}
Fig. 16. Schematic diagram for NI–FEM/NFAM difference schemes (for $\overline{C}_{i,j}^\theta$) from Appendices A and B.

where

$$T_{i,j}^{(1)} = 0,$$

$$T_{i,j}^{(2)} = \frac{g_{i+1,j}^{(4)}}{D} - \frac{g_{i+1,j}^{(2)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}} + \frac{b_{i,j}^2 Pe x_{i,j} htn_{i,j}^{(11)}}{2a_{i,j} \left( a_{i,j}^2 + b_{i,j}^2 \right)} \left( gtn_{i,j}^{(8)} - gtn_{i,j}^{(9)} \right)$$

$$\text{htn}_{i,j}^{(8)} \left( gtn_{i,j}^{(8)} - gtn_{i,j}^{(9)} \right)$$

$$- a_{i,j} \left( gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)} \right)$$

$$+ \frac{2 \left( a_{i,j}^2 + b_{i,j}^2 \right)}{2} \left( gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)} \right),$$

$$T_{i,j}^{(3)} = -\frac{g_{i+1,j}^{(4)}}{D} - \frac{g_{i+1,j}^{(2)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}},$$

$$T_{i,j,k}^{(4)} = 0,$$

$$T_{i,j}^{(5)} = \frac{b_{i,j}^2 Pe x_{i,j} htn_{i,j}^{(11)} gtn_{i,j}^{(9)}}{2a_{i,j} \left( a_{i,j}^2 + b_{i,j}^2 \right)} \left( gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)} \right)$$

$$+ \frac{\text{htn}_{i,j}^{(8)} gtn_{i,j}^{(9)}}{a_{i,j} \left( gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)} \right)}$$

$$+ \frac{a_{i,j} Pe y_{i,j} gtn_{i,j}^{(10)}}{2 \left( a_{i,j}^2 + b_{i,j}^2 \right)} \left( \text{htn}_{i,j}^{(8)} + htn_{i,j}^{(9)} \right)$$

$$+ \frac{\left( htn_{i,j}^{(8)} + htn_{i,j}^{(9)} \right)}{2} \left( gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)} \right),$$

$$T_{i,j}^{(6)} = \frac{h_{i+1,j}^{(1)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}},$$

\[ T_{i,j}^{(7)} = \frac{h_{i+1,j}^{(2)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \]
\[ T_{i,j}^{(8)} = \frac{a_{i,j} b_{i,j}^2}{2(a_{i,j}^2 + b_{i,j}^2)}, \]
\[ T_{i,j}^{(9)} = \frac{h_{i+1,j}^{(3)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \]
\[ T_{i,j}^{(10)} = -\frac{b_{i,j}^2 Pe x_{i,j} htn_{i,j}^{(11)} gtn_{i,j}^{(8)}}{2a_{i,j}(a_{i,j}^2 + b_{i,j}^2)(gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)})} \]
\[ - a_{i,j}(gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)}) \]
\[ - a_{i,j} Pe y_{i,j} gtn_{i,j}^{(10)} htn_{i,j}^{(8)} \]
\[ - 2(a_{i,j}^2 + b_{i,j}^2)(gtn_{i,j}^{(8)} htn_{i,j}^{(8)} - gtn_{i,j}^{(9)} htn_{i,j}^{(8)} + gtn_{i,j}^{(8)} htn_{i,j}^{(9)}). \]

Appendix B. NI–FAM difference scheme for the steady-state convection–diffusion equation

The NI–FAM difference scheme shown below for \( \tilde{C}_{i,j}^\nu \) (see Fig. 16) corresponds to one type of rectangular–triangular node interface. Difference schemes for the additional types of rectangular–triangular node interfaces (see Figs. 2 and 3(a)) are similar and can be easily derived following the approach presented in Section 2.1.3. The coefficients, \( g, h, gtn, \) and \( htn, \) are given in Appendix E.

\[ (F_{i,j}^{(1)})_{i-1,j} + (F_{i,j}^{(2)})_{i,j} + (F_{i,j}^{(3)})_{i+1,j} + (F_{i,j}^{(4)})_{i,j} + (F_{i,j}^{(5)})_{i+1,j} + (F_{i,j}^{(6)})_{i,j} + (F_{i,j}^{(7)})_{i+1,j-1} + (F_{i,j}^{(8)})_{i,j} + (F_{i,j}^{(9)})_{i+1,j} + (F_{i,j}^{(10)})_{i,j} = 0, \]

where

\[ F_{i,j}^{(1)} = 0, \]
\[ F_{i,j}^{(2)} = gtn_{i,j}^{(7)} + g_{i+1,j}^{(4)} - \frac{gtn_{i,j}^{(1)} gtn_{i,j}^{(6)}}{gtn_{i,j}^{(3)} + htn_{i,j}^{(3)}} - \frac{g_{i+1,j}^{(2)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \]
\[ F_{i,j}^{(3)} = -g_{i+1,j}^{(4)} - \frac{g_{i+1,j}^{(1)} g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \]
\[ F_{i,j}^{(4)} = 0, \]
\[ F_{i,j}^{(5)} = \frac{htn_{i,j}^{(2)} gtn_{i,j}^{(6)}}{gtn_{i,j}^{(3)} + htn_{i,j}^{(3)}}, \]
Appendix C. NI–FAM difference scheme for the time-dependent convection–diffusion equation

The NI–FAM difference scheme shown below for $\mathbf{C}_{i,j,k}^t$ (see Fig. 17) corresponds to one type of parallelepiped–wedge-shaped-node interface. Difference schemes for the additional types of interfaces (see Figs. 2 and 3(a)) are similar and can be easily derived following the approach presented in Section 2.2. The coefficients, $g$, $h$, $gtn$, and $htn$, are given in Appendix E.

\begin{align*}
F_{i,j}^{(6)} &= \frac{h_{i+1,j}^{(1)}g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \\
F_{i,j}^{(7)} &= \frac{h_{i+1,j}^{(2)}g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \\
F_{i,j}^{(8)} &= \frac{ht_{i,j}^{(3)}gtn_{i,j}^{(6)}}{gtn_{i,j}^{(3)} + htn_{i,j}^{(3)}}, \\
F_{i,j}^{(9)} &= \frac{h_{i+1,j}^{(3)}g_{i+1,j}^{(5)}}{g_{i+1,j}^{(3)} + h_{i+1,j}^{(3)}}, \\
F_{i,j}^{(10)} &= -gtn_{i,j}^{(7)} - \frac{gtn_{i,j}^{(2)}gtn_{i,j}^{(6)}}{gtn_{i,j}^{(3)} + htn_{i,j}^{(3)}} + \frac{gtn_{i,j}^{(6)}htn_{i,j}^{(1)}}{gtn_{i,j}^{(3)} + htn_{i,j}^{(3)}},
\end{align*}

Fig. 17. Schematic diagram for NI–FAM difference scheme (for $\mathbf{C}_{i,j}^t$) from Appendix C.
where

\[
G_{ij,k}^{(1)} = 0,
\]

\[
G_{ij,k}^{(2)} = g_{n}^{(7)} + g_{n}^{(4)} - \frac{g_{n}^{(1)}g_{n}^{(6)}}{g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(3)} = -g_{n}^{(4)} - \frac{g_{n}^{(1)}g_{n}^{(5)}}{g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(4)} = 0,
\]

\[
G_{ij,k}^{(5)} = \frac{h_{n}^{(2)}g_{n}^{(6)}}{g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(6)} = \frac{h_{n}^{(1)}g_{n}^{(5)}}{g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(7)} = \frac{h_{n}^{(2)}g_{n}^{(5)}}{g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(8)} = \frac{h_{n}^{(2)}g_{n}^{(6)}}{2\tau_{k}g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(9)} = -\frac{h_{n}^{(2)}g_{n}^{(6)}}{2\tau_{k}g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(10)} = \frac{h_{n}^{(1)}g_{n}^{(5)}}{2\tau_{k}g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(11)} = -\frac{h_{n}^{(1)}g_{n}^{(5)}}{2\tau_{k}g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(12)} = \frac{h_{n}^{(2)}g_{n}^{(6)}}{2\tau_{k}g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(13)} = \frac{h_{n}^{(1)}g_{n}^{(5)}}{2\tau_{k}g_{n}^{(3)} + h_{n}^{(3)}},
\]

\[
G_{ij,k}^{(14)} = -g_{n}^{(7)} - \frac{g_{n}^{(2)}g_{n}^{(6)}}{g_{n}^{(3)} + h_{n}^{(3)}} + \frac{g_{n}^{(6)}h_{n}^{(1)}}{g_{n}^{(3)} + h_{n}^{(3)}}.
\]
Appendix D. NI–FAM difference scheme in the time direction for the time-dependent convection–diffusion equation

The NI–FAM discretization scheme shown below for the discrete variable, \( C_{i,j,k}^{xy} \) (see Fig. 18), corresponds to one type of wedge-shaped node. Difference schemes for the additional types of wedge-shaped nodes (see Fig. 3(a)) are similar and can be easily derived following the approach presented in Section 2.2. The coefficients, \( g, h, gtn, \) and \( htn \), are given in Appendix E.

\[
(H_{i,j,k}^{(1)}) C_{i,j,k}^{xy} + (H_{i,j,k}^{(2)}) C_{i,j,k}^{xy} + (H_{i,j,k}^{(3)}) C_{i-1,j,k}^{xt} + (H_{i,j,k}^{(4)}) C_{i,j,k}^{xt} + (H_{i,j,k}^{(5)}) C_{i,j,k+1}^{xt} + (H_{i,j,k}^{(6)}) C_{i,j,k}^{xt} + (H_{i,j,k}^{(7)}) Q_{i,j,k}^{yf} + (H_{i,j,k}^{(8)}) C_{i,j,k}^{ht} = 0,
\]

where

\[
H_{i,j,k}^{(1)} = 1 + \frac{2gtn_{i,j,k}^{(3)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})} + \frac{2htn_{i,j,k}^{(3)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})},
\]

\[
H_{i,j,k}^{(2)} = -1,
\]

\[
H_{i,j,k}^{(3)} = 0,
\]

\[
H_{i,j,k}^{(4)} = - \frac{2gtn_{i,j,k}^{(1)} htn_{i,j,k}^{(3)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})},
\]

\[
H_{i,j,k}^{(5)} = - \frac{2gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(2)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})},
\]

\[
H_{i,j,k}^{(6)} = 0,
\]

\[
H_{i,j,k}^{(7)} = - \frac{2gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})},
\]

\[
H_{i,j,k}^{(8)} = - \frac{2gtn_{i,j,k}^{(2)} htn_{i,j,k}^{(3)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})} - \frac{2gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(1)} \tau_k}{gtn_{i,j,k}^{(3)} htn_{i,j,k}^{(3)} - \tau_k (gtn_{i,j,k}^{(3)} + htn_{i,j,k}^{(3)})}.
\]

Appendix E. Definition of coefficients, \( g, h, gtn, \) and \( htn, \) for the convection–diffusion equation

The coefficients, \( g, h, gtn, \) and \( htn, \) are used in the expressions for \( T, F, G, \) and \( H, \) which appear in Appendices A through D. These coefficients appear in both the steady-state and time-dependent versions of the difference schemes. In the steady-state version, the subscripts remain as \( i, j; \) while in the time-dependent version, these subscripts become \( i, j, k \) to account for the time direction.
$P_{ex_{i,j}} = \frac{u_{i,j}^{xy} a_{i,j}}{D}$, $P_{ey_{i,j}} = \frac{v_{i,j}^{xy} b_{i,j}}{D}$,

$g_{i,j}^{(1)} = \frac{1}{2 P_{ex_{i,j}}} - \frac{1}{\exp(2 P_{ex_{i,j}}) - 1}$, $h_{i,j}^{(1)} = \frac{1}{2 P_{ey_{i,j}}} - \frac{1}{\exp(2 P_{ey_{i,j}}) - 1}$,

$g_{i,j}^{(2)} = 1 - \frac{1}{2 P_{ex_{i,j}}} + \frac{1}{\exp(2 P_{ex_{i,j}}) - 1}$, $h_{i,j}^{(2)} = 1 - \frac{1}{2 P_{ey_{i,j}}} + \frac{1}{\exp(2 P_{ey_{i,j}}) - 1}$,

$g_{i,j}^{(3)} = \frac{a_{i,j}^2}{D(P_{ex_{i,j}})^2} - \frac{a_{i,j}^2}{D P_{ex_{i,j}} - D P_{ex_{i,j}}(\exp(2 P_{ex_{i,j}}) - 1)}$, $h_{i,j}^{(3)} = \frac{b_{i,j}^2}{D(P_{ey_{i,j}})^2} - \frac{b_{i,j}^2}{D P_{ey_{i,j}} - D P_{ey_{i,j}}(\exp(2 P_{ey_{i,j}}) - 1)}$,

$g_{i,j}^{(4)} = \frac{D P_{ex_{i,j}}}{a_{i,j}(\exp(2 P_{ex_{i,j}}) - 1)}$, $h_{i,j}^{(4)} = \frac{D P_{ey_{i,j}}}{b_{i,j}(\exp(2 P_{ey_{i,j}}) - 1)}$,

$g_{i,j}^{(5)} = \frac{a_{i,j}}{P_{ex_{i,j}}} - \frac{2 a_{i,j}}{\exp(2 P_{ex_{i,j}}) - 1}$, $h_{i,j}^{(5)} = \frac{b_{i,j}}{P_{ey_{i,j}}} - \frac{2 b_{i,j}}{\exp(2 P_{ey_{i,j}}) - 1}$,

$g_{i,j}^{(6)} = \frac{2 a_{i,j}}{1 - \exp(-2 P_{ex_{i,j}})} - \frac{a_{i,j}}{P_{ex_{i,j}}}$, $h_{i,j}^{(6)} = \frac{2 b_{i,j}}{1 - \exp(-2 P_{ey_{i,j}})} - \frac{b_{i,j}}{P_{ey_{i,j}}}$.
\[ g_{i,j}^{(7)} = \frac{DPe_{x_{i,j}}}{a_{i,j}(1 - \exp(-2Pe_{x_{i,j}}))}, \quad h_{i,j}^{(7)} = \frac{DPe_{y_{i,j}}}{b_{i,j}(1 - \exp(-2Pe_{y_{i,j}}))}, \]

\[ g_{i,j}^{(1)} = \frac{1}{Pe_{x_{i,j}}} - \frac{1}{\exp(Pe_{x_{i,j}}) - 1}, \quad h_{i,j}^{(1)} = \frac{1}{Pe_{y_{i,j}}} - \frac{1}{\exp(Pe_{y_{i,j}}) - 1}, \]

\[ g_{i,j}^{(2)} = 1 - \frac{1}{Pe_{x_{i,j}}} + \frac{1}{\exp(Pe_{x_{i,j}}) - 1}, \quad h_{i,j}^{(2)} = 1 - \frac{1}{Pe_{y_{i,j}}} + \frac{1}{\exp(Pe_{y_{i,j}}) - 1}, \]

\[ g_{i,j}^{(3)} = \frac{a_{i,j}^2}{D(Pe_{x_{i,j}})^2} - \frac{2a_{i,j}^2}{2DPe_{x_{i,j}}} - \frac{a_{i,j}^2}{DPe_{x_{i,j}}(\exp(Pe_{x_{i,j}}) - 1)}, \quad h_{i,j}^{(3)} = \frac{b_{i,j}^2}{D(Pe_{y_{i,j}})^2} - \frac{2b_{i,j}^2}{2DPe_{y_{i,j}}} - \frac{b_{i,j}^2}{DPe_{y_{i,j}}(\exp(Pe_{y_{i,j}}) - 1)}, \]

\[ g_{i,j}^{(4)} = \frac{DPe_{x_{i,j}}}{a_{i,j}(\exp(Pe_{x_{i,j}}) - 1)}, \quad h_{i,j}^{(4)} = \frac{DPe_{y_{i,j}}}{b_{i,j}(\exp(Pe_{y_{i,j}}) - 1)}, \]

\[ g_{i,j}^{(5)} = \frac{a_{i,j}}{Pe_{x_{i,j}}} - \frac{a_{i,j}}{\exp(Pe_{x_{i,j}}) - 1}, \quad h_{i,j}^{(5)} = \frac{b_{i,j}}{Pe_{y_{i,j}}} - \frac{b_{i,j}}{\exp(Pe_{y_{i,j}}) - 1}, \]

\[ g_{i,j}^{(6)} = \frac{a_{i,j}}{1 - \exp(-Pe_{x_{i,j}})} - \frac{a_{i,j}}{Pe_{x_{i,j}}}, \quad h_{i,j}^{(6)} = \frac{b_{i,j}}{1 - \exp(-Pe_{y_{i,j}})} - \frac{b_{i,j}}{Pe_{y_{i,j}}}, \]

\[ g_{i,j}^{(7)} = \frac{DPe_{x_{i,j}}}{a_{i,j}(1 - \exp(-Pe_{x_{i,j}}))}, \quad h_{i,j}^{(7)} = \frac{DPe_{y_{i,j}}}{b_{i,j}(1 - \exp(-Pe_{y_{i,j}}))}, \]

\[ g_{i,j}^{(8)} = \frac{1 - \exp(2Pe_{x_{i,j}})}{2Pe_{x_{i,j}}}, \quad h_{i,j}^{(8)} = \frac{1 - \exp(2Pe_{y_{i,j}})}{2Pe_{y_{i,j}}}, \]

\[ g_{i,j}^{(9)} = \frac{1 - \exp(2Pe_{x_{i,j}})}{2(2Pe_{x_{i,j}})^2} + \frac{1 + \exp(2Pe_{x_{i,j}})}{2(2Pe_{x_{i,j}})}, \quad h_{i,j}^{(9)} = \frac{1 - \exp(2Pe_{y_{i,j}})}{2(2Pe_{y_{i,j}})^2} + \frac{1 + \exp(2Pe_{y_{i,j}})}{2(2Pe_{y_{i,j}})}, \]

\[ g_{i,j}^{(10)} = \frac{1 - \exp(2Pe_{x_{i,j}})}{2(2Pe_{x_{i,j}})^2} + \frac{\exp(2Pe_{x_{i,j}})}{Pe_{x_{i,j}}}, \quad h_{i,j}^{(10)} = \frac{1 - \exp(2Pe_{y_{i,j}})}{2(2Pe_{y_{i,j}})^2} + \frac{\exp(2Pe_{y_{i,j}})}{Pe_{y_{i,j}}}, \]

\[ g_{i,j}^{(11)} = \frac{1 - \exp(2Pe_{x_{i,j}})}{2(2Pe_{x_{i,j}})^2} + \frac{1}{Pe_{x_{i,j}}}, \quad h_{i,j}^{(11)} = \frac{1 - \exp(2Pe_{y_{i,j}})}{2(2Pe_{y_{i,j}})^2} + \frac{1}{Pe_{y_{i,j}}}. \]
References


