Advanced Heat Transfer

Part IV: Numerical Heat Transfer Methods

3. Convection-Diffusion Problems

(Application of the Finite Volume Method)

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Convection-Diffusion Problems — Outline

1. One-Dimensional (1D) Steady-State Conditions

Governing Equations

- The effects of convection (besides diffusion) must be accounted for whenever fluid flow plays a relevant transport role.
- The corresponding governing equation – the convection-diffusion equation for a general (transported) property ϕ – can be obtained from the general transport equation in a differential form for steady-state conditions by neglecting the transient term as follows

$$\mathrm{div}\,(\rho\phi\mathbf{u}) = \mathrm{div}\,(\Gamma\,\mathrm{grad}\,\phi) + S_\phi$$

- Overall mass conservation must also be respected and, consequently, the following equation (steady-state continuity equation) must be added to the mathematical model formulation.

$$\mathrm{div}\,(\rho\mathbf{u}) = 0$$

- For the current study of simultaneous convection and diffusion transport of ϕ, the flow field ($\mathbf{u}$ and ρ) is assumed to be known (not calculated).

1. 1D Steady-State Conditions

Governing Equations

- For 1D (Cartesian coordinates) and in the absence of sources for property ϕ ($S_\phi = 0$) the following equations govern the steady-state convection and diffusion transport processes of ϕ:

Convection-Diffusion Eq.

$$\frac{d}{dx}(\rho u \phi) = \frac{d}{dx}\left(\Gamma \frac{d\phi}{dx}\right)$$

Continuity Eq.

$$\frac{d}{dx}(\rho u) = 0$$

- The integration of the differential governing equations over a 1D CV at node P that is surrounded by nodes (faces) W (w) and E (e) yields:

Convection-Diffusion Eq.

$$(\rho u A \phi)_\mathrm{e} - (\rho u A \phi)_\mathrm{w} = \left(\Gamma A \frac{d\phi}{dx}\right)_\mathrm{e} - \left(\Gamma A \frac{d\phi}{dx}\right)_\mathrm{w}$$

Continuity Eq.

$$(\rho u A)_\mathrm{e} = (\rho u A)_\mathrm{w}$$

1. 1D Steady-State Conditions

Bulk Control Volumes – Discretized Governing Equations

Considering F and D as the convective mass flux and diffusion conductance, respectively, given by

$$F \equiv \rho u \Rightarrow \begin{cases} F_{\mathrm{w}} = (\rho u)_{\mathrm{w}} \\ F_{\mathrm{e}} = (\rho u)_{\mathrm{e}} \end{cases} \qquad D \equiv \frac{\Gamma}{\delta_x} \Rightarrow \begin{cases} D_{\mathrm{w}} = \frac{\Gamma}{\delta_{x_{\mathrm{WP}}}} \\ D_{\mathrm{e}} = \frac{\Gamma}{\delta_{x_{\mathrm{PE}}}} \end{cases}$$

and since $A_{\mathrm{w}} = A_{\mathrm{e}} = A$, the integration of the convection-diffusion and continuity equations presented before can be written as follows

$$\boxed{F_{\mathrm{e}}\phi_{\mathrm{e}} - F_{\mathrm{w}}\phi_{\mathrm{w}} = D_{\mathrm{e}}\left(\phi_{\mathrm{E}} - \phi_{\mathrm{P}}\right) - D_{\mathrm{w}}\left(\phi_{\mathrm{P}} - \phi_{\mathrm{W}}\right)}$$

$$\boxed{F_{\mathrm{e}} - F_{\mathrm{w}} = 0}$$

The diffusion terms were discretized with the central differencing scheme – as before. No assumption was yet considered for the discretization of the convective terms, particularly, how the transported property ϕ (and its convective flux) is calculated at the CV faces.

1. 1D Steady-State Conditions

Discretized Governing Equations – Convective Term Discretization

- The convective term can be discretized using different schemes. Three schemes are herein considered:
    1. central differencing (CD) scheme;
    2. upwind differencing (UD) scheme; and
    3. hybrid differencing (HD) scheme.
- Note that the flow field is somehow known and not calculated – flow field calculation irrelevant at the moment.

Discretized Governing Equations – Central Differencing Scheme

According to the central differencing approach, the calculation of ϕ_w and ϕ_e is based on linear interpolation between nodes W and P and nodes P and E, respectively. For a uniform grid, this scheme yields:

$$\phi_\mathrm{w} = \frac{\phi_\mathrm{W} + \phi_\mathrm{P}}{2} \qquad \phi_\mathrm{e} = \frac{\phi_\mathrm{P} + \phi_\mathrm{E}}{2}$$

1. 1D Steady-State Conditions

Discretized Governing Equations – Central Differencing Scheme

Substituting the expressions for ϕ_w and ϕ_e obtained with the central differencing scheme in the integrated convection-diffusion equation, we have:

$$F_\mathrm{e}\phi_\mathrm{e} - F_\mathrm{w}\phi_\mathrm{w} = D_\mathrm{e}\left(\phi_\mathrm{E} - \phi_\mathrm{P}\right) - D_\mathrm{w}\left(\phi_\mathrm{P} - \phi_\mathrm{W}\right) \Leftrightarrow$$

$$\frac{F_\mathrm{e}}{2}\left(\phi_\mathrm{P} + \phi_\mathrm{E}\right) - \frac{F_\mathrm{w}}{2}\left(\phi_\mathrm{W} + \phi_\mathrm{P}\right) = D_\mathrm{e}\left(\phi_\mathrm{E} - \phi_\mathrm{P}\right) - D_\mathrm{w}\left(\phi_\mathrm{P} - \phi_\mathrm{W}\right)$$

and re-arranging,

$$\left[\left(D_\mathrm{w} + \frac{F_\mathrm{w}}{2}\right) + \left(D_\mathrm{e} - \frac{F_\mathrm{e}}{2}\right) + \left(F_\mathrm{e} - F_\mathrm{w}\right)\right]\phi_\mathrm{P} =$$

$$\underbrace{\left(D_\mathrm{w} + \frac{F_\mathrm{w}}{2}\right)}_{a_\mathrm{W}}\phi_\mathrm{W} + \underbrace{\left(D_\mathrm{e} - \frac{F_\mathrm{e}}{2}\right)}_{a_\mathrm{E}}\phi_\mathrm{E} \Leftrightarrow$$

$$\underbrace{\left[a_\mathrm{W} + a_\mathrm{E} + \left(F_\mathrm{e} - F_\mathrm{w}\right)\right]}_{a_\mathrm{P}}\phi_\mathrm{P} = a_\mathrm{W}\phi_\mathrm{W} + a_\mathrm{E}\phi_\mathrm{E} \Leftrightarrow \boxed{a_\mathrm{P}\phi_\mathrm{P} = a_\mathrm{W}\phi_\mathrm{W} + a_\mathrm{E}\phi_\mathrm{E}}$$

Note that from the integration of the continuity equation $F_\mathrm{e} - F_\mathrm{w} = 0$ and, consequently, $a_\mathrm{P} = a_\mathrm{W} + a_\mathrm{E}$.

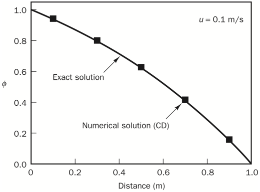
Central Differencing Scheme – Unbounded Solutions

- The application of the central differencing approach to the convective term poses a limitation on the grid size to obtain a bounded solution – compliance with the boundedness property. For a specific convective mass flux (F) and diffusion coefficient (Γ), there are a minimum number of CVs – dictated by the relative strength of convection and diffusion effects – that are required to obtain a stable and accurate solution.
- [Exemplification] Consider the transport of a property ϕ governed by the convection-diffusion equation in the 1D domain $0 \leq x \leq L$. The value of property ϕ is prescribed at both domain boundaries: $\phi(x = 0) = 1$ and $\phi(x = L) = 0$. Considering $L = 1\,\mathrm{m}$, $\rho = 1\,\mathrm{kg\,m^{-3}}$, and $\Gamma = 0.1\,\mathrm{kg\,m^{-1}\,s^{-1}}$, determine the numerical solution obtained with the central differencing (CD) method for the following cases:
  1. $u = 0.1\,\mathrm{m\,s^{-1}}$ with 5 equally distributed cells;
  2. $u = 2.5\,\mathrm{m\,s^{-1}}$ with 5 equally distributed cells; and
  3. $u = 2.5\,\mathrm{m\,s^{-1}}$ with 20 equally distributed cells.

Central Differencing Scheme – Unbounded Solutions

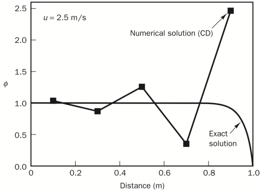
- The following figure presents the comparison between the numerical solution (symbols) and analytical solution (solid line) for the three cases.

Case 1



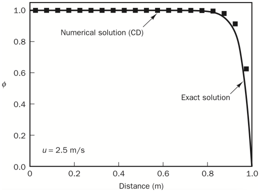
$u = 0.1\,\mathrm{m\,s^{-1}}$ and $\delta_x = 0.2\,\mathrm{m}$

Case 2



$u = 2.5\,\mathrm{m\,s^{-1}}$ and $\delta_x = 0.2\,\mathrm{m}$

Case 3



$u = 2.5\,\mathrm{m\,s^{-1}}$ and $\delta_x = 0.05\,\mathrm{m}$

- The combination of grid parameters (cell spacing) and fluid and flow properties (ρ, Γ, and u) of Case 2 leads to unrealistic (unbounded) solution with oscillations characterized by large under- and overshoots – solution containing wiggles.
- The evidence that the boundedness criterion is violated for Case 2 (and not for Cases 1 and 3) is justified by the sign of the coefficients (a_{W}, a_{P}, and a_{E}) of the discretized equations – see next slide.

1. 1D Steady-State Conditions

Central Differencing Scheme – Unbounded Solutions

- According to the boundedness property – that all discretization schemes should respect – all coefficients of the discretized equations should have the same sign (positive). The conditions for which this property is respected are calculated as follows:

$$\left\{\begin{array}{l} a_{\mathrm{W}} > 0 \\ a_{\mathrm{E}} > 0 \end{array}\right. \Leftrightarrow \left\{\begin{array}{l} D_{\mathrm{w}} + \frac{F_{\mathrm{w}}}{2} > 0 \\ D_{\mathrm{e}} - \frac{F_{\mathrm{e}}}{2} > 0 \end{array}\right. \Leftrightarrow \left\{\begin{array}{l} Pe_{\mathrm{w}} \equiv \frac{F_{\mathrm{w}}}{D_{\mathrm{w}}} > -2 \\ Pe_{\mathrm{e}} \equiv \frac{F_{\mathrm{e}}}{D_{\mathrm{e}}} < 2 \end{array}\right. \Leftrightarrow |Pe| < 2$$

- To avoid wiggles (unbounded solution) the cell Peclet number, Pe, should be below 2 because otherwise the coefficients a_{W} and a_{E} have different signs.
- Case 2 does not respect the boundedness property since $Pe > 2$ (see below), and consequently, the coefficient of ϕ_{E} will be negative – *i.e.*, $a_{\mathrm{E}} < 0$. (For Cases 1 and 3, the coefficients a_{W}, a_{P}, and a_{E} have a positive sign. Note that if a_{W} and a_{E} are positive a_{P} $(= a_{\mathrm{W}} + a_{\mathrm{E}})$ is also positive.)

$$Pe = Pe_{\mathrm{w}} = Pe_{\mathrm{e}} = \frac{F}{D} = \frac{\rho u \delta_x}{\Gamma} = \left\{\begin{array}{ll} 0.20, & \text{Case 1} \\ 5.00, & \text{Case 2} \\ 1.25, & \text{Case 3} \end{array}\right.$$

1. 1D Steady-State Conditions

Central Differencing Scheme – Unbounded Solutions

- To obtain a bounded (physically realistic) solution – *i.e.*, to avoid the violation of the boundedness property that is observed if $|Pe| > 2$ – the cell spacing, δx, should be kept below a maximum value. (The maximum cell spacing value is dictated by fluid properties and flow conditions.)
  - As a consequence, for convection-diffusion problems where convection effects are more relevant than diffusion transport steps, a very large number of CVs, and, consequently, a high computational cost is required to obtain a bounded solution.

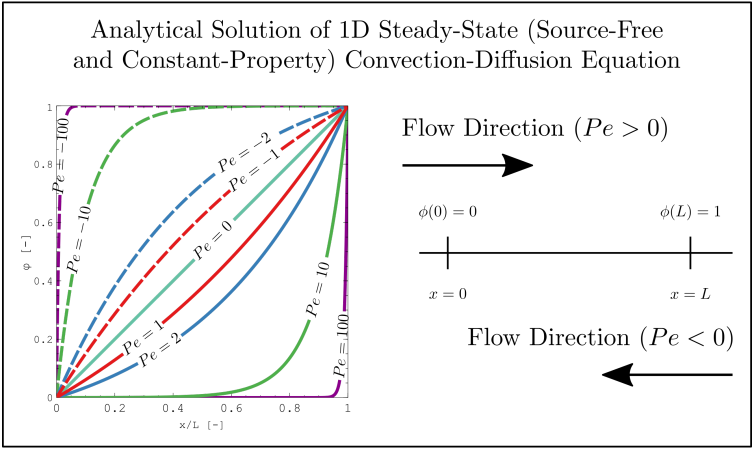
Transportiveness (1/3)

- Transportiveness (besides conservativeness and boundedness) is a property that discretization schemes applied to convection-diffusion problems should possess.

1. 1D Steady-State Conditions

Transportiveness (2/3)

- The transportiveness property can be perceived with the analytical solution of the 1D convection-diffusion equation.

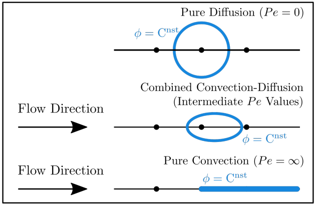


1. 1D Steady-State Conditions

Transportiveness (3/3)

- At a particular location (for instance at $x/L = 0.5$), the influence of upstream conditions increases (in relation to downstream) as the relative importance of convection over diffusion ($|Pe|$) increases.
- For pure diffusion conditions – stagnant fluid – ($Pe = 0$) a linear profile is obtained which means that transport rates are independent of direction.
- Transportiveness property can also be recognized with the figure below:
  - for pure diffusion, a similar influence of a property source is observed independently of direction; and
  - for simultaneous convection and diffusion transport, the source influence on neighboring nodes becomes biased taking into account the flow direction and the magnitude of Peclet number.

Isolines of ϕ in the Vicinity of the ϕ Source Point Location for Different Dominant Transp. Mechanisms



1. 1D Steady-State Conditions

Central Differencing Scheme – Transportiveness (Lack of)

- The central differencing approach applied to the convective term does not allow to take into consideration the flow direction or the relative importance of convection over diffusion, and consequently, this discretization scheme does not exhibit transportiveness. (Applying the central differencing scheme, all neighboring nodes exert an effect on a central node P independently of the flow direction and magnitude of Peclet number.)
- The lack of transportiveness – as well as the inability to produce bounded (realistic) solutions for large values of the cell Peclet number – hinders the application of the central differencing schemes for general purpose convection-diffusion problems. Therefore, other convective discretization schemes should be introduced – see next slides.

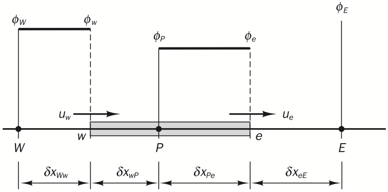
1. 1D Steady-State Conditions

Discretized Governing Equations – Upwind Differencing Scheme

The upwind scheme – contrarily to the central differencing scheme – takes into account the flow direction for the determination of the property ϕ value at the cell face: the convected value of ϕ at a cell face is considered equal to the value of the upstream node.

Flow in Positive Direction,

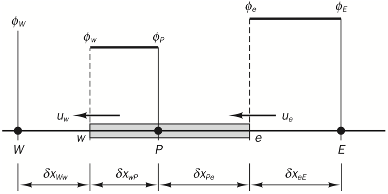
$$u = u_{\mathrm{w}} = u_{\mathrm{e}} > 0$$
$$(F = F_{\mathrm{w}} = F_{\mathrm{e}} > 0)$$



$$\phi_{\mathrm{w}} = \begin{cases} \phi_{\mathrm{W}} & \text{if } F > 0 \\ \phi_{\mathrm{P}} & \text{if } F < 0 \end{cases}$$

Flow in Negative Direction,

$$u = u_{\mathrm{w}} = u_{\mathrm{e}} < 0$$
$$(F = F_{\mathrm{w}} = F_{\mathrm{e}} < 0)$$



$$\phi_{\mathrm{e}} = \begin{cases} \phi_{\mathrm{P}} & \text{if } F > 0 \\ \phi_{\mathrm{E}} & \text{if } F < 0 \end{cases}$$

1. 1D Steady-State Conditions

Discretized Governing Equations – Upwind Differencing Scheme

Taking into account the definition for ϕ_{w} and ϕ_{e} presented in the previous slide, the convective terms $F_{\mathrm{e}}\phi_{\mathrm{e}}$ and $F_{\mathrm{w}}\phi_{\mathrm{w}}$ discretized according to the upwind differencing method are given as follows:

$$F_{\mathrm{e}}\phi_{\mathrm{e}} = \phi_{\mathrm{P}} \max\left(F_{\mathrm{e}}, 0\right) - \phi_{\mathrm{E}} \max\left(-F_{\mathrm{e}}, 0\right)$$

$$F_{\mathrm{w}}\phi_{\mathrm{w}} = \phi_{\mathrm{W}} \max\left(F_{\mathrm{w}}, 0\right) - \phi_{\mathrm{P}} \max\left(-F_{\mathrm{w}}, 0\right)$$

$$\begin{aligned}
F_{\mathrm{e}}\phi_{\mathrm{e}} - F_{\mathrm{w}}\phi_{\mathrm{w}} = D_{\mathrm{e}}\left(\phi_{\mathrm{E}} - \phi_{\mathrm{P}}\right) - D_{\mathrm{w}}\left(\phi_{\mathrm{P}} - \phi_{\mathrm{W}}\right) \Leftrightarrow \\
\left[\phi_{\mathrm{P}} \max\left(F_{\mathrm{e}}, 0\right) - \phi_{\mathrm{E}} \max\left(-F_{\mathrm{e}}, 0\right)\right] - \left[\phi_{\mathrm{W}} \max\left(F_{\mathrm{w}}, 0\right) - \phi_{\mathrm{P}} \max\left(-F_{\mathrm{w}}, 0\right)\right] = \\
D_{\mathrm{e}}\left(\phi_{\mathrm{E}} - \phi_{\mathrm{P}}\right) - D_{\mathrm{w}}\left(\phi_{\mathrm{P}} - \phi_{\mathrm{W}}\right) \Leftrightarrow \left\{\left[D_{\mathrm{w}} + \max\left(-F_{\mathrm{w}}, 0\right)\right] + \left[D_{\mathrm{e}} + \max\left(F_{\mathrm{e}}, 0\right)\right]\right\}\phi_{\mathrm{P}} = \\
\left[D_{\mathrm{w}} + \max\left(F_{\mathrm{w}}, 0\right)\right]\phi_{\mathrm{W}} + \left[D_{\mathrm{e}} + \max\left(-F_{\mathrm{e}}, 0\right)\right]\phi_{\mathrm{E}} \Leftrightarrow \\
\left\{\left[D_{\mathrm{w}} + \max\left(F_{\mathrm{w}}, 0\right)\right] + \left[D_{\mathrm{e}} + \max\left(-F_{\mathrm{e}}, 0\right)\right] + \left(F_{\mathrm{e}} - F_{\mathrm{w}}\right)\right\}\phi_{\mathrm{P}} = \\
\left[D_{\mathrm{w}} + \max\left(F_{\mathrm{w}}, 0\right)\right]\phi_{\mathrm{W}} + \left[D_{\mathrm{e}} + \max\left(-F_{\mathrm{e}}, 0\right)\right]\phi_{\mathrm{E}} \Rightarrow \ldots \text{ Next Slide}
\end{aligned}$$

1. 1D Steady-State Conditions

Discretized Governing Equations – Upwind Differencing Scheme

$$\text{Prev. Slide} \Rightarrow \left\{ [D_w + \max(F_w, 0)] + [D_e + \max(-F_e, 0)] + (F_e - F_w) \right\} \phi_P = \underbrace{[D_w + \max(F_w, 0)]}_{a_W} \phi_W + \underbrace{[D_e + \max(-F_e, 0)]}_{a_E} \phi_E \Leftrightarrow$$

$$\underbrace{[a_W + a_E + (F_e - F_w)]}_{a_P} \phi_P = a_W \phi_W + a_E \phi_E \Leftrightarrow \boxed{a_P \phi_P = a_W \phi_W + a_E \phi_E}$$

Note that from the integration of the continuity equation $F_e - F_w = 0$ and, consequently, $a_P = a_W + a_E$.

1. 1D Steady-State Conditions

Upwind Differencing Scheme – Accuracy

- The upwind differencing scheme is based on the backward differencing expression and, consequently, its Taylor series truncation error (TSTE) is of first-order.
    - Note that according to the upwind scheme, the net convective flux is given by the following equation

$$F^c \equiv \int_{x_\mathrm{w}}^{x_\mathrm{e}} \frac{d}{dx} (F\phi)\, dx = F_\mathrm{e}\phi_\mathrm{e} - F_\mathrm{w}\phi_\mathrm{w} = F\left(\phi_\mathrm{e} - \phi_\mathrm{w}\right) \Leftrightarrow F^c = F\left(\phi_\mathrm{P} - \phi_\mathrm{W}\right)$$

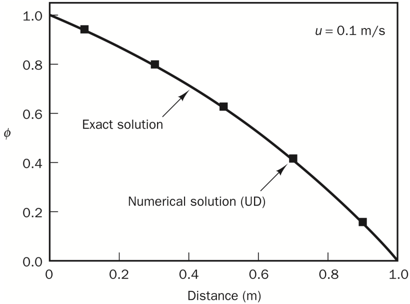
    The same result would be obtained if $d\left(F\phi\right)/dx$ were substituted by $F\left(\phi_\mathrm{P} - \phi_\mathrm{W}\right)/\Delta x$. Consequently, the upwind discretization scheme is based on a first-order (backward) differencing scheme.

1. 1D Steady-State Conditions

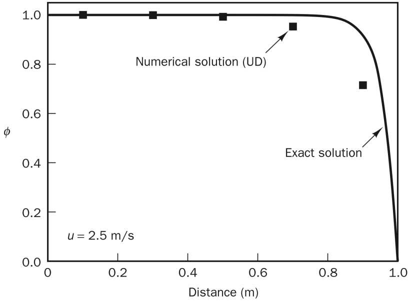
Upwind Differencing Scheme – Performance

Cases 1 and 2 (see Slide 8 *et seq.*) were again solved considering the upwind scheme applied to the convective term – see results below.

Case 1



Case 2

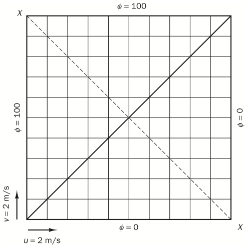


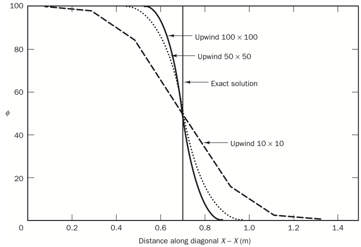
- Since the upwind scheme complies with the boundedness criterion (positive coefficients and matrix of coefficients diagonally dominant) the obtained results are physically realistic.

1. 1D Steady-State Conditions

Upwind Differencing Scheme – False Diffusion

- The application of the upwind differencing scheme in multi-dimensional problems leads to spurious (erroneous) results when the flow is not aligned with the grid lines. The corresponding error is commonly referred to as false diffusion.
- An example of false diffusion for a 2D steady problem is shown below (left – physical model and right – results). In this problem, no source is considered and the transport of ϕ is exclusively controlled by convection. However, the results falsely suggest the existence of diffusion by a smooth (and not abrupt) profile transition from $\phi = 100$ to $\phi = 0$ where the the diagonal lines meet each other.





1. 1D Steady-State Conditions

Discretized Governing Equations – Hybrid Differencing Scheme

- The hybrid differencing scheme is a combination of the central and upwind differencing approaches.
  - For $|Pe| < 2$, the central differencing scheme is considered for the diffusive and convective terms; and
  - for $|Pe| \geq 2$, the upwind scheme is applied for the convective term and the diffusion term is set to zero.

$$\underbrace{\left[a_{\mathrm{W}} + a_{\mathrm{E}} + (F_{\mathrm{e}} - F_{\mathrm{w}})\right]}_{a_{\mathrm{P}}} \phi_{\mathrm{P}} = a_{\mathrm{W}}\phi_{\mathrm{W}} + a_{\mathrm{E}}\phi_{\mathrm{E}} \Leftrightarrow \boxed{a_{\mathrm{P}}\phi_{\mathrm{P}} = a_{\mathrm{W}}\phi_{\mathrm{W}} + a_{\mathrm{E}}\phi_{\mathrm{E}}}$$

$$a_{\mathrm{W}} = \max\left[F_{\mathrm{w}}, \left(D_{\mathrm{w}} + \frac{F_{\mathrm{w}}}{2}\right), 0\right] \qquad a_{\mathrm{E}} = \max\left[-F_{\mathrm{e}}, \left(D_{\mathrm{e}} - \frac{F_{\mathrm{e}}}{2}\right), 0\right]$$

Note that from the integration of the continuity equation $F_{\mathrm{e}} - F_{\mathrm{w}} = 0$ and, consequently, $a_{\mathrm{P}} = a_{\mathrm{W}} + a_{\mathrm{E}}$.

1. 1D Steady-State Conditions

Hybrid Differencing Scheme

- The upwind scheme overestimates the diffusion transport contribution for high $|Pe|$ – note that the diffusion term is discretized considering a linear profile (see the figure in Slide 12 for $Pe = 0$) and such interpolation assumption fails strongly when $|Pe|$ is large for which $d\phi/dx$ is negligible at $x/L = 0.5$. This issue is solved with the hybrid scheme.
- The hybrid scheme is unconditionally bounded – since the coefficients are always positive – and it satisfies the transportiveness criterion.
- The hybrid scheme yields physically realistic solutions.

Discretization Schemes – Summary of Properties

Property	Discretization Scheme		
	Central Differ.	Upwind Differ.	Hybrid Differ.
Conservativeness	✓	✓	✓
Boundedness	Only for $\lvert Pe\rvert < 2$	✓	✓
Transportiveness	✗	✓	✓
Accuracy – TSTE	2^{nd} Order	1^{st} Order	$1^{\text{st}}/2^{\text{nd}}$ Order

2. Multi-Dimensional (MD) Problems

2D Unsteady Governing Equations

In 2D (two-dimensional Cartesian coordinates), transient convection and diffusion transport processes of a property ϕ are governed by the following equations:

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial}{\partial x}(\rho u\phi)+\frac{\partial}{\partial y}(\rho v\phi)=\frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma\frac{\partial\phi}{\partial y}\right)+S_\phi$$

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}(\rho u)+\frac{\partial}{\partial y}(\rho v)=0$$

The first equation corresponds to the convection-diffusion equation for property ϕ and the second equation corresponds to the continuity equation. The convection-diffusion equation can be written as

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial(J_x)}{\partial x}+\frac{\partial(J_y)}{\partial y}=S_\phi$$

where J_x and J_y correspond to the total flux (convective and diffusive) defined by

$$J_x=\rho u\phi-\Gamma\frac{\partial\phi}{\partial x}\qquad\qquad J_y=\rho v\phi-\Gamma\frac{\partial\phi}{\partial y}$$

2. MD Problems

Bulk Control Volumes – Discretized 2D Unsteady Governing Equations

The integration and temporal discretization with the fully implicit scheme of the 2D unsteady convection-diffusion and continuity equations yield the following two equations. (The superscript "1" used previously to denote properties at time $t+\Delta t$ is hereafter not considered.)

$$\frac{\left(\rho_{\mathrm{P}}\phi_{\mathrm{P}}-\rho_{\mathrm{P}}^{0}\phi_{\mathrm{P}}^{0}\right)\Delta x\Delta y\cdot 1}{\Delta t}+\left(J_{\mathrm{e}}-J_{\mathrm{w}}\right)+\left(J_{\mathrm{n}}-J_{\mathrm{s}}\right)=\left(s_{\mathrm{C}}+s_{\mathrm{P}}\phi_{\mathrm{P}}\right)\Delta x\Delta y\cdot 1$$

$$\frac{\left(\rho_{\mathrm{P}}-\rho_{\mathrm{P}}^{0}\right)\Delta x\Delta y\cdot 1}{\Delta t}+\left(F_{\mathrm{e}}-F_{\mathrm{w}}\right)+\left(F_{\mathrm{n}}-F_{\mathrm{s}}\right)=0$$

For convenience, the subtraction of the LHS of the last equation (integration of the continuity equation) multiplied by ϕ_{P} from the LHS of discretized convection-diffusion equation lead to:

$$\frac{\rho_{\mathrm{P}}^{0}\left(\phi_{\mathrm{P}}-\phi_{\mathrm{P}}^{0}\right)\Delta x\Delta y\cdot 1}{\Delta t}+\left[\left(J_{\mathrm{e}}-F_{\mathrm{e}}\phi_{\mathrm{P}}\right)-\left(J_{\mathrm{w}}-F_{\mathrm{w}}\phi_{\mathrm{P}}\right)\right]+\left[\left(J_{\mathrm{n}}-F_{\mathrm{n}}\phi_{\mathrm{P}}\right)-\left(J_{\mathrm{s}}-F_{\mathrm{s}}\phi_{\mathrm{P}}\right)\right]=S_{\mathrm{C}}+S_{\mathrm{P}}\phi_{\mathrm{P}}$$

2. MD Problems

Bulk Control Volumes – Discretized 2D Unsteady Governing Equations

The second term on the LHS of the previous equation can be written as follows

$$J_e - F_e\phi_P = \left(\rho u\phi - \Gamma\frac{\partial\phi}{\partial x}\right)_e \Delta y \cdot 1 - F_e\phi_P =$$

$$F_e\phi_e - \Gamma_e\frac{\phi_E - \phi_P}{\delta_{x_{PE}}}\Delta y \cdot 1 - F_e\phi_P = F_e\left(\phi_e - \phi_P\right) - D_e\left(\phi_E - \phi_P\right)$$

where $F_e = (\rho u)_e\,\Delta y \cdot 1$ and $D_e = (\Gamma_e\Delta y \cdot 1)/\delta_{x_{PE}}$. The grid Peclet number is defined as $Pe_e = F_e/D_e = \left[(\rho u)_e\,\delta_{x_{PE}}\right]/\Gamma_e$. According to the hybrid diff. scheme:

$$J_e - F_e\phi_P = \begin{cases} F_e\left(\phi_E - \phi_P\right) & Pe_e \leq -2 \\ \left(F_e/2 - D_e\right)\left(\phi_E - \phi_P\right) & -2 < Pe_e < 2 \\ 0 & Pe_e \geq 2. \end{cases}$$

The last equation can be written as

$$J_e - F_e\phi_P = \underbrace{\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]}_{a_E}\left(\phi_P - \phi_E\right)$$

2. MD Problems

Bulk Control Volumes – Discretized 2D Unsteady Governing Equations

The third term on the LHS of the last equation of Slide 24 can be written as follows

$$J_\mathrm{w} - F_\mathrm{w}\phi_\mathrm{P} = \left(\rho u \phi - \Gamma \frac{\partial \phi}{\partial x}\right)_\mathrm{w} \Delta y \cdot 1 - F_\mathrm{w}\phi_\mathrm{P} =$$

$$F_\mathrm{w}\phi_\mathrm{w} - \Gamma_\mathrm{w} \frac{\phi_\mathrm{P} - \phi_\mathrm{W}}{\delta_{x_\mathrm{WP}}} \Delta y \cdot 1 - F_\mathrm{w}\phi_\mathrm{P} = F_\mathrm{w}\left(\phi_\mathrm{w} - \phi_\mathrm{P}\right) - D_\mathrm{w}\left(\phi_\mathrm{P} - \phi_\mathrm{W}\right)$$

where $F_\mathrm{w} = (\rho u)_\mathrm{w} \Delta y \cdot 1$ and $D_\mathrm{w} = (\Gamma_\mathrm{w} \Delta y \cdot 1)/\delta_{x_\mathrm{WP}}$. The grid Peclet number is defined as $Pe_\mathrm{w} = F_\mathrm{w}/D_\mathrm{w} = \left[(\rho u)_\mathrm{w} \delta_{x_\mathrm{WP}}\right]/\Gamma_\mathrm{w}$. According to the hybrid diff. scheme:

$$J_\mathrm{w} - F_\mathrm{w}\phi_\mathrm{P} = \begin{cases} 0 & Pe_\mathrm{w} \leq -2 \\ \left(F_\mathrm{w}/2 + D_\mathrm{w}\right)\left(\phi_\mathrm{W} - \phi_\mathrm{P}\right) & -2 < Pe_\mathrm{w} < 2 \\ F_\mathrm{w}\left(\phi_\mathrm{W} - \phi_\mathrm{P}\right) & Pe_\mathrm{w} \geq 2. \end{cases}$$

The last equation can be written as

$$J_\mathrm{w} - F_\mathrm{w}\phi_\mathrm{P} = \underbrace{\max\left[F_\mathrm{w}, \left(D_\mathrm{w} + \frac{F_\mathrm{w}}{2}\right), 0\right]}_{a_\mathrm{W}} \left(\phi_\mathrm{W} - \phi_\mathrm{P}\right)$$

2. MD Problems

Bulk Control Volumes – Discretized 2D Unsteady Governing Equations

Analogously, the fourth and fifth terms on the LHS of the last equation in Slide 24 can be written as follows

$$J_n - F_n\phi_P = \underbrace{\max\left[-F_n, \left(D_n - \frac{F_n}{2}\right), 0\right]}_{a_N}(\phi_P - \phi_N)$$

$$J_s - F_s\phi_P = \underbrace{\max\left[F_s, \left(D_s + \frac{F_s}{2}\right), 0\right]}_{a_S}(\phi_S - \phi_P)$$

where, $F_n = (\rho v)_n \Delta x \cdot 1$, $F_s = (\rho v)_s \Delta x \cdot 1$, $D_n = (\Gamma_n \Delta x \cdot 1)/\delta_{y_{PN}}$, and $D_s = (\Gamma_s \Delta x \cdot 1)/\delta_{y_{SP}}$.

Substituting the expressions obtained for $J_e - F_e\phi_P$, $J_w - F_w\phi_P$, $J_s - F_s\phi_P$, and $J_n - F_n\phi_P$ into the last equation of Slide 24, one obtains the following equation

$$\frac{\rho_P^0\left(\phi_P - \phi_P^0\right)\Delta x \Delta y \cdot 1}{\Delta t} + a_E(\phi_P - \phi_E) - a_W(\phi_W - \phi_P) + a_S(\phi_P - \phi_S) - a_N(\phi_N - \phi_P) = S_C + S_P\phi_P$$

2. MD Problems

Bulk Control Volumes – Discretized 2D Unsteady Governing Equations

The last equation of previous slide can be written in a compact form as follows:

$$a_{\mathrm{P}}\phi_{\mathrm{P}} = \sum_{\mathrm{nb}} a_{\mathrm{nb}}\phi_{\mathrm{nb}} + b$$

where,

$$a_{\mathrm{P}} = \sum_{\mathrm{nb}} a_{\mathrm{nb}} + \rho_{\mathrm{P}}^{0}\frac{\Delta x \Delta y}{\Delta t} - S_{\mathrm{P}} \qquad b = \frac{\rho_{\mathrm{P}}^{0}\Delta x \Delta y}{\Delta t}\phi_{\mathrm{P}}^{0} + S_{\mathrm{C}}$$

$$a_{\mathrm{E}} = \max\left[-F_{\mathrm{e}}, \left(D_{\mathrm{e}} - \frac{F_{\mathrm{e}}}{2}\right), 0\right] \qquad a_{\mathrm{W}} = \max\left[F_{\mathrm{w}}, \left(D_{\mathrm{w}} + \frac{F_{\mathrm{w}}}{2}\right), 0\right]$$

$$a_{\mathrm{N}} = \max\left[-F_{\mathrm{n}}, \left(D_{\mathrm{n}} - \frac{F_{\mathrm{n}}}{2}\right), 0\right] \qquad a_{\mathrm{S}} = \max\left[F_{\mathrm{s}}, \left(D_{\mathrm{s}} + \frac{F_{\mathrm{s}}}{2}\right), 0\right]$$

2. MD Problems

3D Unsteady Governing Equations

In 3D (three-dimensional Cartesian coordinates), the unsteady convection-diffusion equation for a property ϕ reads as follows:

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x}(\rho u\phi) + \frac{\partial}{\partial y}(\rho v\phi) + \frac{\partial}{\partial z}(\rho w\phi) =$$
$$\frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma\frac{\partial\phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\Gamma\frac{\partial\phi}{\partial z}\right) + S_\phi$$

2. MD Problems

Bulk Control Volumes – Discretized 3D Unsteady Governing Equations

The discretized 3D unsteady convection-diffusion equation for an internal nodal point P, considering the fully implicit scheme for the temporal discretization and the hybrid scheme for the spatial discretization reads as follows:

$$a_{\mathrm{P}}\phi_{\mathrm{P}} = \sum_{\mathrm{nb}} a_{\mathrm{nb}}\phi_{\mathrm{nb}} + b$$

where,

$$a_{\mathrm{P}} = \sum_{\mathrm{nb}} a_{\mathrm{nb}} + \rho_{\mathrm{P}}^{0}\frac{\Delta x \Delta y \Delta z}{\Delta t} - S_{\mathrm{P}} \qquad b = \frac{\rho_{\mathrm{P}}^{0}\Delta x \Delta y \Delta z}{\Delta t}\phi_{\mathrm{P}}^{0} + S_{\mathrm{C}}$$

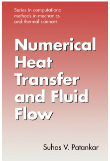
$$a_{\mathrm{T}} = \max\left[-F_{\mathrm{t}}, \left(D_{\mathrm{t}} - \frac{F_{\mathrm{t}}}{2}\right), 0\right] \qquad a_{\mathrm{B}} = \max\left[F_{\mathrm{b}}, \left(D_{\mathrm{b}} + \frac{F_{\mathrm{b}}}{2}\right), 0\right]$$

The expressions to evaluate the coefficients a_{E}, a_{W}, a_{N}, and a_{S} presented in Slide 28 still hold for the 3D case. The mass flow rates (1) and conductances (2) at the east, north, and top CV faces are computed as follows: (1) $F_{\mathrm{e}} = (\rho u)_{\mathrm{e}}\Delta y \Delta z$, $F_{\mathrm{n}} = (\rho v)_{\mathrm{n}}\Delta x \Delta z$, and $F_{\mathrm{t}} = (\rho w)_{\mathrm{t}}\Delta x \Delta y$; and (2) $D_{\mathrm{e}} = (\Gamma_e \Delta y \Delta z)/\delta_{x_{\mathrm{PE}}}$, $D_{\mathrm{n}} = (\Gamma_n \Delta x \Delta z)/\delta_{y_{\mathrm{PN}}}$, and $D_{\mathrm{t}} = (\Gamma_t \Delta x \Delta y)/\delta_{z_{\mathrm{PT}}}$.

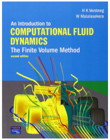
Suggested Problem:

Problem 11

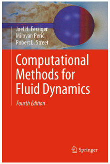
Further Reading



- Chapter 5: Convection and Diffusion



- Chapter 5: The Finite Volume Method for Convection-Diffusion Problems



- Chapter 4: Finite Volume Methods