Computational Fluid Dynamics
Exercise II

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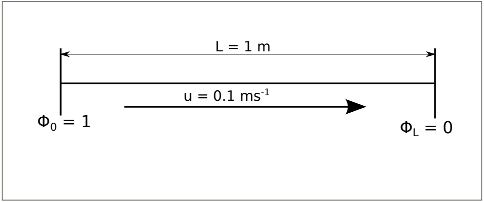
LSM

Problem 1: 1-D Convection-Diffusion

A property ϕ is transported by means of convection and diffusion through the 1-D domain sketched in below figure. Using five equally spaced cells and the central difference scheme for convection and diffusion, calculate the distribution of ϕ.

The following data apply:

- $\rho = 1.0 kgm^{-3}$
- $\Gamma = 0.1 kgm^{-1}s^{-1}$
- $Pe = \frac{\delta x \mathbf{u} \rho}{\Gamma} = 0.2$



Solution 1: 1-D Convection-Diffusion

1. Identify the governing equation for the problem

$$\frac{\partial \rho\phi}{\partial t} + \nabla \cdot (\rho\phi\mathbf{u}) = \nabla \cdot (\Gamma\nabla\phi) + \mathbf{S}_\phi \qquad (1)$$

1. Identify the governing equation for the problem

$$\underbrace{\cancel{\frac{\partial \rho \phi}{\partial t}}}_{\text{steady state}} + \nabla \cdot (\rho \phi \mathbf{u}) = \nabla \cdot (\Gamma \nabla \phi) + \underbrace{\cancel{\mathbf{S}_\phi}}_{\text{no source}}$$

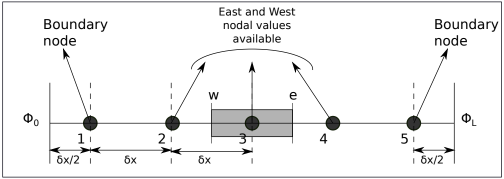
$$\nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi)$$

2. Discretize the domain

1. Identify the governing equation for the problem

$$\nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) \tag{2}$$

2. Discretize the domain



3. Discretized convective part,
   I Apply Gauss divergence theorem,

$$\int_V \nabla \cdot (\rho \mathbf{u} \phi) dV = \oint_S (\rho \mathbf{u} \phi) \cdot d\mathbf{S} \tag{3}$$

$$\mathbf{S} = S\mathbf{n} \tag{4}$$

   II Rewrite surface integral for faces,

$$\oint_S (\rho \mathbf{u} \phi) \cdot \mathbf{S} = \sum_f^{n_f} \int_S (\rho \mathbf{u} \phi \cdot \mathbf{n})_f \cdot dS_f \tag{5}$$

   III Apply Gauss quadrature rule,

$$\sum_f^{n_f} \int_S (\rho \mathbf{u} \phi \cdot \mathbf{n})_f \cdot S_f = \sum_f^{n_f} \sum_{ip}^{n_{ip}} (\rho \mathbf{u} \phi \cdot \mathbf{n})_{ip,f} \omega_{ip} \cdot S_f \tag{6}$$

$$n_{ip} = 1,\ \omega_{ip} = 1 \tag{7}$$

3. Discretization of the convective part,
   - III Apply Gauss quadrature rule,

$$\sum_{f}^{n_f} \int_{S} (\rho \mathbf{u} \phi \cdot \mathbf{n})_f \cdot S_f = \sum_{f}^{n_f} (\rho \mathbf{u} \phi \cdot \mathbf{n})_f \cdot S_f \tag{8}$$

Face flux $F_f = (\rho \mathbf{u} \cdot \mathbf{n})_f$

   - IV Linear interpolate ϕ at the faces (Central difference scheme),

$$\phi_f = \frac{\phi_N - \phi_P}{x_N - x_P}(x_f - x_P) + \phi_P \tag{9}$$

For a equidistant grid,

$$\phi_f = \frac{\phi_N + \phi_P}{2} \tag{10}$$

N Neighbour
P Owner

3. Discretization of the convective part,
   - V Final discretized form,

$$\int_V \nabla \cdot (\rho \mathbf{u} \phi) dV \approx \sum_f^{n_f} F_f \phi_f S_f \tag{11}$$

What happens if $\mathbf{u}$ is not a const. vector field?

4. Discretization of the diffusive part,

$$\int_V \nabla \cdot (\Gamma \nabla \phi) dV \approx \sum_f^{n_f} \Gamma_f (\nabla \phi \cdot \mathbf{n})_f S_f \tag{12}$$

see previous exercise ...

Solution 1: 1-D Convection-Diffusion

5. Discretize inner node 3,
   - $\mathbf{u}$, ρ is const. $|F_e| = |F_w| = ... = F$
   - Γ is const.
   - $S_e = S_w = ... = S$

   For the convective part,

$$\sum_f^{n_f} F_f \phi_f S_f = \frac{FS}{2}(\phi_4 - \phi_2) \tag{13}$$

remember

$$\mathbf{n}_e = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \text{ and } \mathbf{n}_w = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}$$

5. Discretize inner node 3,
   - II For the diffusive part,

$$(\nabla\phi\cdot\mathbf{n})_e = \begin{bmatrix}\frac{\partial\phi}{\partial x}\\ \frac{\partial\phi}{\partial y}\\ \frac{\partial\phi}{\partial z}\end{bmatrix}_e \cdot \begin{bmatrix}1\\0\\0\end{bmatrix} = \left(\frac{\partial\phi}{\partial x}\right)_e$$

$$(\nabla\phi\cdot\mathbf{n})_w = \begin{bmatrix}\frac{\partial\phi}{\partial x}\\ \frac{\partial\phi}{\partial y}\\ \frac{\partial\phi}{\partial z}\end{bmatrix}_w \cdot \begin{bmatrix}-1\\0\\0\end{bmatrix} = -\left(\frac{\partial\phi}{\partial x}\right)_w$$

$$\left(\frac{\partial\phi}{\partial x}\right)_e = \frac{\phi_4-\phi_3}{\underbrace{x_4-x_3}_{\delta x}} \text{ and } \left(\frac{\partial\phi}{\partial x}\right)_w = \frac{\phi_3-\phi_2}{\underbrace{x_3-x_2}_{\delta x}} \tag{14}$$

Solution 1: 1-D Convection-Diffusion

5. Discretize inner node 3,
   - II For the diffusive part,

$$\sum_{f}^{n_f} \Gamma_f (\nabla\phi \cdot \mathbf{n})_f S_f = \frac{\Gamma S}{\delta x}(\phi_4 - 2\phi_3 + \phi_2) \tag{15}$$

$$D = \frac{\Gamma}{\delta x}$$

   - III Set eq. (13) = eq. (15),

$$\frac{F\cancel{S}}{2}(\phi_4 - \phi_2) = D\cancel{S}(\phi_4 - 2\phi_3 + \phi_2) \tag{16}$$

5. Discretize inner node 3,
   III Set eq. (13) = eq. (15),

$$\underbrace{\left(\frac{F}{2} - D\right)}_{-0.45\,\frac{kg}{m^2 s}} \phi_4 + \underbrace{2D}_{1\,\frac{kg}{m^2 s}} \phi_3 - \underbrace{\left(\frac{F}{2} + D\right)}_{-0.55\,\frac{kg}{m^2 s}} \phi_2 = 0 \qquad (17)$$

6. Discretize for the boundaries,
   I node 1,

$$\Gamma\left(\frac{\phi_2 - \phi_1}{\delta x} - \frac{\phi_1 - \phi_0}{\frac{\delta x}{2}}\right) = \frac{F}{2}(\phi_2 + \phi_1) - F\phi_0 \qquad (18)$$

$$D\left(\phi_2 - 3\phi_1 + 2\phi_0\right) = \frac{F}{2}(\phi_2 + \phi_1) - F\phi_0 \qquad (19)$$

Solution 1: 1-D Convection-Diffusion

6. Discretize for the boundaries
   I node 1,

$$\underbrace{(3D + \frac{F}{2})}_{1.55\,\frac{kg}{m^2 s}} \phi_1 + \underbrace{(\frac{F}{2} - D)}_{-0.45\,\frac{kg}{m^2 s}} \phi_2 = \underbrace{(2D + F)}_{1.1\,\frac{kg}{m^2 s}} \phi_0 \tag{20}$$

   II node 5,

$$\underbrace{(3D - \frac{F}{2})}_{1.45\,\frac{kg}{m^2 s}} \phi_5 \underbrace{-(D + \frac{F}{2})}_{-0.55\,\frac{kg}{m^2 s}} \phi_4 = \underbrace{-(F + 2D)}_{-1.1\,\frac{kg}{m^2 s}} \cancel{\phi_L} \tag{21}$$

7. Build the discretized matrix,

$$\begin{bmatrix} 1.55 & -0.45 & 0 & 0 & 0 \\ -0.55 & 1.0 & -0.45 & 0 & 0 \\ 0 & -0.55 & 1.0 & -0.45 & 0 \\ 0 & 0 & -0.55 & 1.0 & -0.45 \\ 0 & 0 & 0 & -0.55 & 1.45 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 1.1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

8. Solving the linear system of equations,

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 0.9421 \\ 0.8006 \\ 0.6276 \\ 0.4163 \\ 0.1579 \end{bmatrix}$$

9. Compare to the analytical solution,

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{e^{\rho \mathbf{u} x/\Gamma} - 1}{e^{\rho \mathbf{u} L/\Gamma} - 1} \tag{22}$$

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 0.9387 \\ 0.7963 \\ 0.6224 \\ 0.4100 \\ 0.1505 \end{bmatrix}$$

$$rel.error[\%] = \begin{bmatrix} -0.36 \\ -0.53 \\ -0.83 \\ -1.53 \\ -4.91 \end{bmatrix}$$

Problem 2: 1-D Convection-Diffusion

Repeat problem 1 for a velocity $\mathbf{u} = 2.5ms^{-1}$.

i Compare the Pecelt number with the previous task. What is the dominating term?

ii Does the numerical solution matches with the analytical solution when using the central difference scheme (CDS)?

iii Instead of using the CDS try to use the upwind difference scheme (UDS).

iv Compare the solution obtained from the UDS to the analytical and the CDS solution.

v What are the advantages and disadvantages of the UDS compared to the CDS?

ii CDS and analytical solution

- Solution for ϕ using CDS,

$$\begin{bmatrix}\phi_1\\\phi_2\\\phi_3\\\phi_4\\\phi_5\end{bmatrix} = \begin{bmatrix}1.0356\\0.8694\\1.2573\\0.3521\\2.4644\end{bmatrix}$$

- Analytical solution,

$$\begin{bmatrix}\phi_1\\\phi_2\\\phi_3\\\phi_4\\\phi_5\end{bmatrix} = \begin{bmatrix}1.0000\\0.9999\\0.9999\\0.9994\\0.9179\end{bmatrix}$$

iii Using Upwind difference scheme for interpolating ϕ at the faces,

- If $u_w > 0, u_e > 0 (F_w > 0, F_e > 0)$

$$\phi_w = \phi_W \text{ and } \phi_e = \phi_P \tag{23}$$

- If $u_w < 0, u_e < 0 (F_w < 0, F_e < 0)$

$$\phi_w = \phi_P \text{ and } \phi_e = \phi_E \tag{24}$$

- Equation (11) becomes for point 3,

$$\sum_f^{n_f} F_f \phi_f S_f = FS(\phi_P - \phi_W) = FS(\phi_3 - \phi_2) \tag{25}$$

iii Using Upwind difference scheme for interpolating ϕ at the faces,

- For point 3,

$$-(F+D)\phi_2 + (F+2D)\phi_3 - D\phi_4 = 0 \tag{26}$$

- For point 1

$$(F+3D)\phi_1 - D\phi_2 = (F+2D)\phi_0 \tag{27}$$

- For point 5

$$(F-D)\phi_4 + (-F+3D)\phi_5 = 2D\phi_L \tag{28}$$

Solution 1: 1-D Convection-Diffusion

- Build the discretized matrix,

$$\begin{bmatrix} 4 & -0.5 & 0 & 0 & 0 \\ -3 & 3.5 & -0.5 & 0 & 0 \\ 0 & -3 & 3.5 & -0.5 & 0 \\ 0 & 0 & -3 & 3.5 & -0.5 \\ 0 & 0 & 0 & -3 & 4 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 3.5 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- Solving the linear system of equations,

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 0.9998 \\ 0.9987 \\ 0.9921 \\ 0.9524 \\ 0.7143 \end{bmatrix}$$

iv UDS and analytical solution

- Analytical solution,

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 1.0000 \\ 0.9999 \\ 0.9999 \\ 0.9994 \\ 0.9179 \end{bmatrix}$$

$$rel.error[\%] = \begin{bmatrix} 0.0 \\ 0.01 \\ 0.7 \\ 4.7 \\ 20.15 \end{bmatrix}$$