Lecture 15
APPLICATIONS OF FDM TO SCALAR TRANSPORT PROBLEMS

15.1 ONE DIMENSIONAL HEAT CONDUCTION

Let us consider steady state heat conduction in a slab of width L with thermal conductivity k and heat generation q_g. The governing equation for this problem is

$$k\frac{\partial^2 T}{\partial x^2}+q_g=0 \tag{15.1}$$

Suppose that the left end of the slab is maintained at constant temperature and the right end of the slab is losing heat by convection to surroundings. Thus, boundary conditions are

$$T(0)=\overline{T} \tag{15.2}$$

$$-k\left.\frac{dT}{dx}\right|_{x=L}=h\left(T-T_a\right) \tag{15.3}$$

where $\overline{T}$ is specified temperature, h is convection heat transfer coefficient and T_a is ambient temperature.

For finite difference formulation, let us use a uniform grid of size $\Delta x=L/N$ where N denotes the number of divisions in the grid. Thus, there are (N+1) grid points. Using CDS for approximation of the second order derivative, discretized form of Eq. (15.1) at an internal node $x=x_i$ becomes

$$\frac{T_{i+1}+T_{i-1}-2T_i}{\Delta x^2}+\frac{q_{g,i}}{k}=0 \quad \text{or} \quad -T_{i-1}+2T_i-T_{i+1}=\frac{q_{g,i}\Delta x^2}{k} \tag{15. 4}$$

Using the matrix notation introduced in the previous section, the preceding equation can be written as

$$A_{\mathrm{P}}^i T_{\mathrm{P}}+A_{\mathrm{W}}^i T_{i-1}+A_{\mathrm{E}}^i T_{i+1}=Q_i \qquad (i=2,3,..,N) \tag{15.5}$$

where $A_{\mathrm{P}}^i=2,\quad A_{\mathrm{W}}^i=A_{\mathrm{E}}^i=-1,$ and $Q_i=q_{gi}\Delta x^2/k.$

At the left boundary node $(i=1)$, $T_1\equiv T(0)=\overline{T}$. Hence, $A_{\mathrm{P}}^1=1,\ A_{\mathrm{W}}^1=A_{\mathrm{E}}^1=0,$ and $Q_1=T_a$. At the right boundary node $(i=N+1)$, use of a backward difference approximation (say, first order BDS) yields

$$-k\frac{T_{N+1}-T_N}{\Delta x}=h\left(T_{N+1}-T_a\right) \quad \text{i.e.} \ -\frac{k}{h\Delta x}T_N+\left(1+\frac{k}{h\Delta x}\right)T_{N+1}=T_a \tag{15.6}$$

Thus, $A_{\mathrm{P}}^{N+1}=1+k/(h\Delta x), A_{\mathrm{E}}^{N+1}=0, A_{\mathrm{W}}^{N+1}=-k/(h\Delta x)$ and $Q_N=T_a$. The linear algebraic system obtained for this problem is tri-diagonal and can be easily solved using TDMA (tri-diagonal matrix algorithm) discussed in a later section.

15.2 TWO DIMENSIONAL HEAT CONDUCTION

Steady state heat conduction in a two dimensional domain without heat source or sink is governed by Laplace equation

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=0 \tag{15.7}$$

Governing equation (15.7) involves second order derivatives which can be approximated using central difference scheme. Associated boundary conditions may involve first order derivatives (in case Neumann or convective boundary conditions), which would require the use of one-sided difference formula.

Using of central difference scheme based on a five point computational molecule yields the following discretized form of Eq. (15.7):

$$\frac{T_{i+1,j}+T_{i-1,j}-2T_{ij}}{\Delta x^2}+\frac{T_{i,j+1}+T_{i,j-1}-2T_{ij}}{\Delta y^2}=0 \tag{15.8}$$

which can be rewritten as

$$A_{\mathrm{P}}T_{\mathrm{P}}+A_{\mathrm{E}}T_{\mathrm{E}}+A_{\mathrm{W}}T_{\mathrm{W}}+A_{\mathrm{N}}T_{\mathrm{N}}+A_{\mathrm{S}}T_{\mathrm{S}}=Q_{\mathrm{P}} \tag{15.9}$$

where $A_{\mathrm{P}}=2/\Delta x^2+2/\Delta y^2, A_{\mathrm{E}}=A_{\mathrm{W}}=-1/\Delta x^2, A_{\mathrm{N}}=A_{\mathrm{S}}=-1/\Delta y^2$ and $Q_{\mathrm{P}}=0$. Discretized equations for boundary nodes can be written using the approach used in 1-D heat conduction problem discussed earlier. The resulting linear algebraic system is penta-diagonal, and can be solved using a suitable direct solver (e.g. Gaussian elimination) or an iterative solver (SOR, conjugate gradient etc.).

15.3 ONE DIMENSIONAL ADVECTION-DIFFUSION

One dimensional advection-diffusion problem for a scalar variable ϕ is governed by

$$\frac{d}{dx}(\rho u\phi)=\frac{d}{dx}\left[\Gamma\frac{d\phi}{dx}\right] \tag{15.10}$$

where u is specified velocity, ρ is density, and Γ is diffusivity. Suppose values of ϕ are specified at both ends of the domain of length L, i.e. the boundary conditions are

$$\phi(0)=\phi_0 \qquad \text{and} \qquad \phi(L)=\phi_L \tag{15.11}$$

Let us employ a non-uniform grid with a total of N+1 grid points (nodes 1 and N+1 represent the boundary nodes $x=0$ and $x=L$ respectively) for finite difference solution of this problem. We can discretize Eq. (15.10) using finite difference scheme based on a there point computational molecule. The resulting discretized equation for an interior node i can be represented as

$$A_{\mathrm{P}}^i\phi_{\mathrm{P}}+A_{\mathrm{W}}^i\phi_{i-1}+\phi_{\mathrm{E}}^iT_{i+1}=Q_i \qquad (i=2,3,..,N) \tag{15.12}$$

where coefficients A contain contributions from both the convective and diffusive terms, i.e. $A = A^d + A^c$ (in which superscripts d and c indicate contribution from diffusive and convective terms respectively).

Central difference scheme (CDS) is commonly used for approximation of the diffusive term (for inner as well as the outer derivative). Thus,

$$\frac{d}{dx}\left[\Gamma\frac{d\phi}{dx}\right]_i \approx \frac{\left(\Gamma\frac{d\phi}{dx}\right)_{i+\frac{1}{2}} - \left(\Gamma\frac{d\phi}{dx}\right)_{i-\frac{1}{2}}}{\frac{1}{2}(x_{i+1}-x_{i-1})} \approx \frac{\Gamma_{i+\frac{1}{2}}\frac{\phi_{i+1}-\phi_i}{x_{i+1}-x_i} - \Gamma_{i-\frac{1}{2}}\frac{\phi_i-\phi_{i-1}}{x_i-x_{i-1}}}{\frac{1}{2}(x_{i+1}-x_{i-1})} \tag{15.13}$$

Therefore, contributions of the diffusive term to the coefficients of algebraic equation (15.12) are

$$A_{\mathrm{E}}^d = \frac{2\Gamma_{i+\frac{1}{2}}}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}, \quad A_{\mathrm{W}}^d = \frac{2\Gamma_{i-\frac{1}{2}}}{(x_{i+1}-x_{i-1})(x_i-x_{i-1})}, \quad A_{\mathrm{P}}^d = -\left(A_{\mathrm{E}}^d + A_{\mathrm{W}}^d\right) \tag{15.14}$$

If the convection term is also discretized using CDS, then

$$\left[\frac{d}{dx}(\rho u\phi)\right]_i \approx \frac{(\rho u\phi)_{i+1} - (\rho u\phi)_{i-1}}{x_{i+1}-x_{i-1}} \tag{15.15}$$

and its contributions to the coefficients of Eq. (15.12) are

$$A_{\mathrm{E}}^c = \frac{(\rho u)_{i+1}}{x_{i+1}-x_{i-1}}, \quad A_{\mathrm{W}}^c = -\frac{(\rho u)_{i-1}}{x_{i+1}-x_{i-1}}, \quad A_{\mathrm{P}}^c = 0 \tag{15.26}$$

Use of CDS for convective term can result in spurious wiggles or oscillations in numerical solution if the local Peclet number, Pe $(=\rho u\Delta x/\Gamma) > 2$. To reduce/eliminate these oscillations, upwind difference is usually employed for convective term. However, first order upwind scheme (based on FDS/BDS) is highly diffusive. Hence, higher order TVD (total variation diminishing schemes) should be preferred for discretization of the convective terms (Versteeg and Malalasekera, 2007; Chung, 2010).

Example 15.1

Consider the steady state heat conduction in a slab of width l = 0.5 m with heat generation. The left end of the slab (x = 0) is maintained at T = 373 K. The right end of the slab (x = 0.5 m) is being heated by a heater for which the heat flux is 1 kW/m^2. The heat generation in the slab is temperature dependent and is given by Q = (1273 – T) W/m^3**.** Thermal conductivity is constant at k = 1 W/(m-K).Write down the governing equation and boundary conditions for the problem. Use the finite difference method (central difference scheme) to obtain an approximate numerical solution of the problem. For the first order derivative, use forward or backward difference approximation of first order. Choose Δx = 0.1, and **use the TDMA.**

Solution

Governing equation for the steady state heat conduction with constant heat generation:

$$k\frac{\mathrm{d}^2T}{\mathrm{d}x^2} + Q = 0 \tag{i}$$

Given: Q = 1273 – T. Thus, Eq. (i) becomes

$$k\frac{\mathrm{d}^2T}{\mathrm{d}x^2} - T = -1273 \tag{ii}$$

Left end of the slab is maintained at constant temperature; hence

$$T(0) = 373 \quad \text{(iii)}$$

At the right end, heat influx is specified. Thus, boundary condition at this end is

$$k\frac{\mathrm{d}T}{\mathrm{d}x} = 1000 \quad \text{(iv)}$$

Using central difference scheme, the discretized form of (ii) at an internal node $x = x_i$ can be expressed as

$$\frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta x^2} - T_i = -1273 \quad \text{(v)}$$

Using given values of $k = 1$ and $\Delta x = 0.1$, the preceding equation simplifies to

$$-T_{i-1} + 2.01T_i - T_{i+1} = 12.73, \quad i = 2,3,4,5 \quad \text{(vi)}$$

Hence, the coefficients in the standard equation $A_W^i T_{i-1} + A_P^i T_i + A_E^i T_{i+1} = b_i$ are:

$$A_W^i = -1,\ A_P^i = 2.01, \quad A_E^i = -1, \quad b_i = 12.73, \quad i = 2,3,4,5 \quad \text{(vii)}$$

Temperature boundary condition (iii) at the first node implies

$$T_1 = 373,\ \text{i.e.}\ A_W^1 = 0,\ A_P^1 = 1, \quad A_E^1 = 0, \quad b_1 = 373 \quad \text{(viii)}$$

Discretization of the flux boundary (iv) requires use of backward difference, which yields

$$T_6 - T_5 = 100,\ \text{i.e.}\ A_W^6 = -1,\ A_P^6 = 1, \quad A_E^6 = 0, \quad b_6 = 100 \quad \text{(ix)}$$

Therefore, the discrete system obtained from finite difference discretization is

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2.01 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2.01 & -1 & 0 & 0 \\ 0 & 0 & 0 & 2.01 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2.01 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{Bmatrix} = \begin{Bmatrix} 373 \\ 12.73 \\ 12.73 \\ 12.73 \\ 12.73 \\ 100 \end{Bmatrix} \quad \text{(x)}$$

Numerical calculations using TDMA are given in the following table:

i	A_W^i	A_P^i	A_E^i	b_i	$A_P^i \leftarrow A_P^i - \frac{A_W^i A_E^{i-1}}{A_P^{i-1}}$	$b_i^* = b_i - \frac{A_W^i b_{i-1}^*}{A_P^{i-1}}$	$T_i = \frac{b_i^* - A_E^i T_{i+1}}{A_P^i}$	T_{ex}
1	0	1.00	0	373	1	373	373.0000	373.00
2	-1	2.01	-1	12.73	2.01	385.73	497.2893	498.95
3	-1	2.01	-1	12.73	1.512487	204.6355	613.8216	617.18
4	-1	2.01	-1	12.73	1.34883754	148.02734	723.7617	728.85
5	-1	2.01	-1	12.73	1.26862087	122.47438	828.2096	835.08
6	-1	1.00	0	100	0.21174243	196.54136	928.2096	936.92

REFERENCES

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Versteeg, H. K. and Malalasekera, W. M. G. (2007). *Introduction to Computational Fluid Dynamics: The Finite Volume Method*. Second Edition (Indian Reprint) Pearson Education.