AKJ

→ Bioreactor :

Biomass ⇒ mass of living organism

Substrate ⇒ feed for growth of biomass

substrate + nutrition ⇒ medium [for ~~treatment of waste water~~]

Raw material (waste water)

↓

Pre-treatment

↓

Reactor ≡ hydrolysis
~~biotransformation~~
biosynthesis
Biodegradation

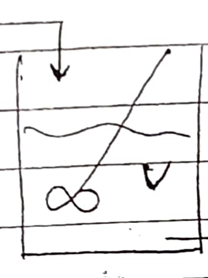
↓

Down stream processing → Flotation, filtering, adsorption, leaching, drying, crystallisation, extraction, distillation

↓

packaging

F, x_f, S_f



x = mass of cells / vol

S ⇒ mass of sub / vol.

→ F, x, S (product is biomass)

Assumption:

1. Perfect mixing
2. Isothermal
3. Feed is sterile
4. ρ constant
5. Single strain for biomass [platensis]

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in − out + gen. = acc.

$$\cancel{\frac{d\rho F}{dt}} = \frac{dv}{dt} = 0$$

$V = const.$

Monod model
↓

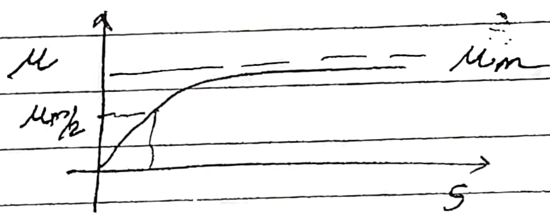
Biomass component balance,

$$Fx_f - Fx + r_A V = \frac{d(Vx)}{dt} \quad \Big| \quad r_A = r_1 = \mu x$$

Substrate component balance,

$$FS_f - FS + (-r_S V) = \frac{d(SV)}{dt}$$

$\mu \Rightarrow$ specific growth rate $= \dfrac{\mu_m S}{k_m + S}$



$$\frac{\mu_m}{2} = \frac{\mu_m S}{k_m + S}$$

$$k_m + S = 2S$$

$$\boxed{k_m = S}$$

yield $= \dfrac{r_1}{r_2}$

$$r_2 = \frac{\mu x}{Y}$$

$$\therefore \frac{dx}{dt} = \frac{F}{V}(x_f - x) + \mu x$$

$D = F/V$ = dilution rate.

maximind

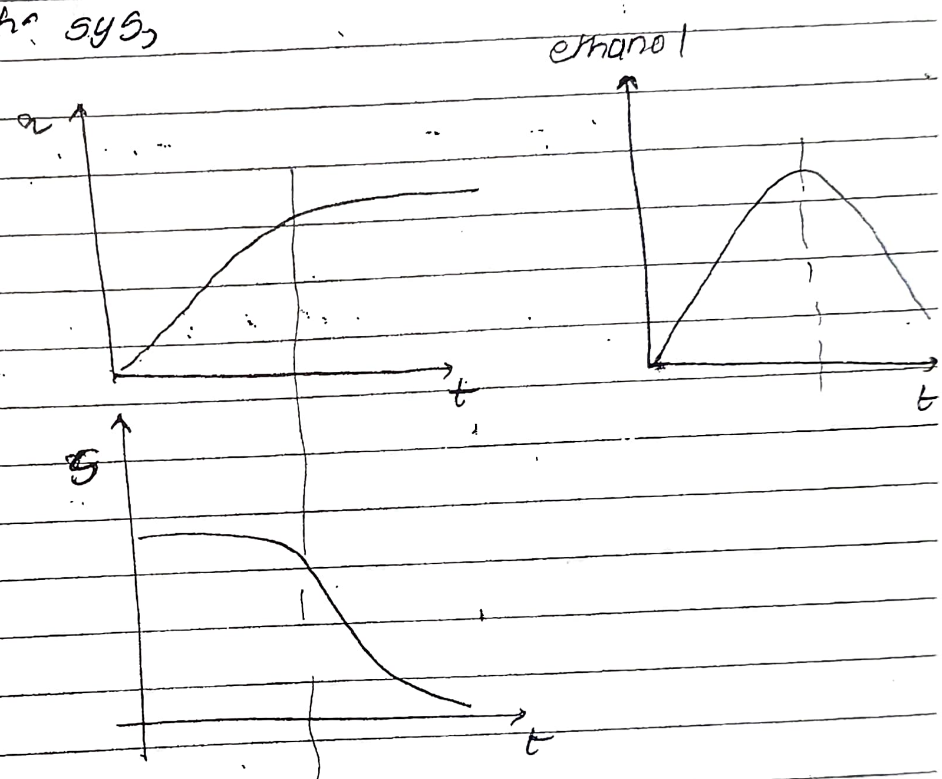
$$\frac{dx}{dt} = (\mu - D)x. \quad (\text{for } x_f = 0)$$

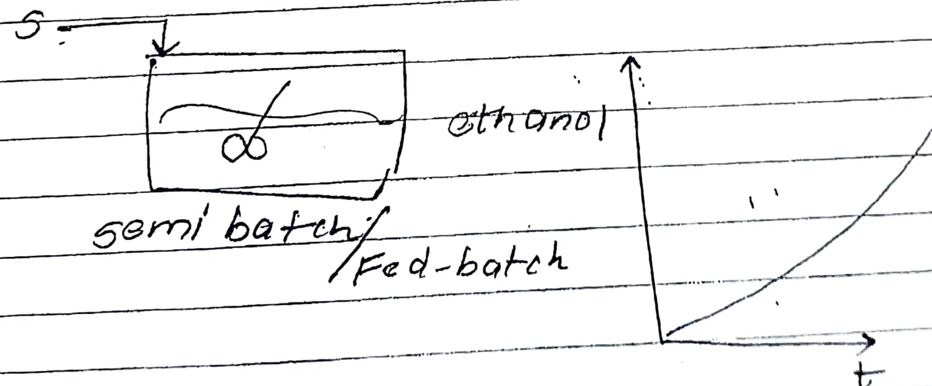
$$\frac{dS}{dt} = D(S_f - S) - \frac{\mu x}{Y}$$

$$\mu = \frac{\mu_m S}{K_m + S}$$

3 eqns ⇒ 1 algebraic & 2 ODE } DAE system.

for batch sys,





⇒ Flow process is rare bcz reaction time is hig.

ODE–BVP

→ Boundary conditions types : 1. Dirichlet BC

$y(x_0) = \beta_1$

$y(x_M) = \beta_2$

2 → Neumann BC.

$\left.\frac{dy}{dx}\right|_{x_0} = \beta$ [ex. no flux condition impermeable membrane]

3 → Robin BC.

$\beta_1 \left.\frac{dy}{dx}\right|_{x_0} + \beta_2 y(x_0) = \beta_3$ ---- combinatⁿ of 1 & 2

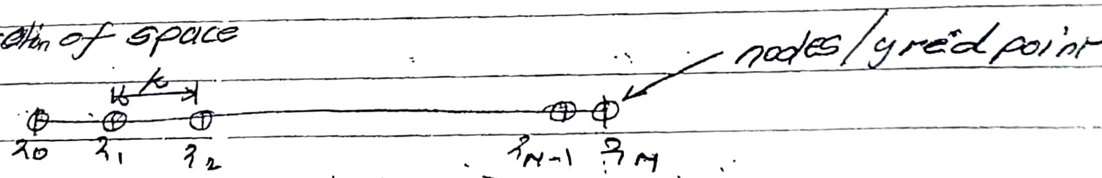
→ Methods:

- Finite difference method
- Initial value method (shooting method)
- Finite element method.
- Orthogonal Collocation

→ FDM:

An approximation of a derivative made in terms of values ~~at~~ at a discrete set of points is called finite difference approximation. The method which is used to perform this approxⁿ is called as FDM.

1. Discretization of space



$x_m = x_0 + mk.$

$m = 0, 1, 2, 3, ---- M$

$k = \frac{x_M - x_0}{M}$ [Mesh size or spatial increment]

total nodes = $M+1$

Derivation:

$$y_{m+1} = y(x_m + \Delta x) = y_m + \Delta x\, y'(x_m) + \frac{\Delta x^2}{2}\frac{d^2y}{dx^2}\Big|_{x=x_m} + O(\Delta x^3) \quad -① $$

$$y_{m+1} = y_m + k\frac{dy}{dx}\Big|_{x=x_m} + O(k^2)$$

$$\frac{dy}{dx}\Big|_{x=x_m} = \frac{y_{m+1} - y_m}{k} + O(k)$$ --- Forward diff. eqn / 2 point Forward diff method.

- 1 order accurate.

$$y_{m-1} = y(x_m - \Delta x) = y_m - \Delta x\frac{dy}{dx}\Big|_{x=x_m} + \frac{\Delta x^2}{2}\times\frac{d^2y}{dx^2}\Big|_{x=x_m} + O(\Delta x^3) \quad -②$$

$$y_{m-1} = y(x_m - \Delta x) = y_m - \Delta x\, dy/dx\Big|_{x=x_m} + O(k^2)$$

$$dy/dx\Big|_{x=x_m} = \frac{y_m - y_{m-1}}{k} + O(k)$$ --- Backward difference eqn

- 1 order accurate

① − ②

$$y_{m+1} - y_{m-1} = 2\Delta x\left(dy/dx\Big|_{x=x_m}\right) + O(\Delta x^3)$$

$$\frac{y_{m+1} - y_{m-1}}{2k} + O(k^2) = dy/dx\Big|_{x=x_m}$$ --- central difference method for 1st order derivative.

- 2 order accurate

① + ②

$$y_{m+1} + y_{m-1} = 2y_m + \Delta x^2\frac{d^2y}{dx^2}\Big|_{x=x_m} + O(\Delta x^4)$$

$$\cancel{\frac{y_{m+1} + y_{m-1} - 2y_m}{k^2}}$$

$$\frac{d^2y}{dx^2}\Big|_{x=x_m} = \frac{-2y_m + y_{m+1} + y_{m-1}}{k^2} + O$$

--- central difference for 2nd order derivative.

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$x_0, x_M \Rightarrow$ boundary nodes

$x_0 \quad x_1 \quad x_2 \quad \ldots \quad x_{M-1} \quad x_M$

$x_1, x_2, \ldots x_{M-1} \Rightarrow$ internal / interior nodes

→ Algorithm:

Step 1: Spatial discretisation

Step 2: Discretize ODE [ODE → set of AE (algebraic eqn)]

no. of AE = $\boxed{M-1}$

Pb: $P(x)\dfrac{d^2y}{dx^2} + q(x)\dfrac{dy}{dx} = r(x)$

BCs: $y(x_0) = y_a \qquad y(x_M) = y_b$

Step 3: Dirichlet BC. $y(m=0)$, $y(m=M)$ @ given

Other: 2 AEs (ODE) ↳ discretise them

@ $M+1$ AE

$M+1$ unknowns $(y_0, y_1, \ldots y_M)$

Remarks: system (ODE) @ non-linear then transformed AEs @ non-linear.

⇒ system: $p(x)\dfrac{d^2y}{dx^2} + q(x)\dfrac{dy}{dx} = r(x)$

use central difference method.

$$\left.\frac{dy}{dx}\right|_{x=x_m} = \frac{y_{m+1} - y_{m-1}}{2h} + O(h^2)$$

$$\left.\frac{d^2y}{dx^2}\right|_{x=x_m} = \frac{2y_m - y_{m+1} - y_{m-1}}{h^2} + O(h^2)$$

$$\therefore\ P(x)\left[\frac{2y_m - y_{m+1} - y_{m-1}}{h^2} + O(h^2)\right] + q(x)\left[\frac{y_{m+1} - y_{m-1}}{2h} + O(h^2)\right] = r(x)$$

$$y_{m-1}\left[\frac{P(x)}{h^2} - \frac{q(x)}{2h}\right] + \left[\frac{2P(x)}{h^2}\right]y_m + O(h^2) = r(x)$$

$$+\ y_{m+1}\left[\frac{+P(x)}{h^2} + \frac{q(x)}{2h}\right]$$

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$$\left[\frac{p(x_m)}{h^2} - \frac{q(x_m)}{2h}\right] y_{m-1} + \left[\frac{-2p(x_m)}{h^2}\right] y_m + \left[\frac{+p_m}{h^2} + \frac{q_m}{2h}\right] y_{m+1} + O(h^2) = r_m$$

$$[2p_m - q_m h]\, y_{m-1} + [-4p_m]\, y_m + [2p_m + q_m h]\, y_{m+1} + O(h^4) = r_m \times 2h^2$$

$m = 1, 2, \ldots, M-1$

$$(2p_1 - q_1 h) y_0 + [-4p_1] y_1 + [2p_1 + q_1 h] y_2 = r_1 \times 2h^2$$

$$(2p_2 - q_2 h) y_1 + [-4p_2] y_2 + [2p_2 + q_2 h] y_3 = r_2 \times 2h^2$$

$\vdots$

$$(2p_{M-1} - q_{M-1} h) y_{M-2} + [-4p_{M-1}] y_{M-1} + [2p_{M-1} + q_{M-1} h] y_M = r_{M-1} \times 2h^2$$

$$\underbrace{\begin{bmatrix} -4p_1 & [2p_1+q_1h] & 0 & \cdots & \\ (2p_2-q_2h) & [-4p_2] & [2p_2+q_2h] & 0 & \cdots \\ & & & & \\ & & & & \\ \cdots & & 0 & (2p_{M-1}-q_{M-1}h) & (-4p_{M-1}) \end{bmatrix}}_{M-1 \times M-1} \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{M-1} \\ \cancel{y_M} \end{bmatrix}}_{M-1 \times 1} = \underbrace{\begin{bmatrix} r_1 2h^2 - (2p_1 - q_1 h) y_0 \\ r_2 \times 2h^2 \\ \vdots \\ r_{M-1} \times 2h^2 - y_M [2p_{M-1} + q_{M-1} h] \end{bmatrix}}_{M-1 \times 1}$$

→ Homework $\quad -\frac{d^2\theta}{dx^2} = 2 \quad x \in [0, 1]$

$M = 6$

center difference

$U(x=0) = 0$

$U(x=1) = 0$

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$$x_M - x_0 / M$$

$$k = \frac{1-0}{6} = 1/6$$

$$\frac{y_{m+1} + y_{m-1} - 2y_m}{k^2} = \left.\frac{d^2y}{dx^2}\right|_{x=x_m}$$

$$\therefore \quad U_{m+1} + U_{m-1} - 2U_m = -2k^2$$

$$U_{m-1} - 2U_m + U_{m+1} = -2k^2$$

$$m \in \{1, \ldots, M-1$$

$$\underset{M-1 \times M-1}{\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}} \underset{M-1 \times 1}{\begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{bmatrix}} = \underset{M-1 \times 1}{\begin{bmatrix} -2k^2 - U_0 \\ -2k^2 \\ -2k^2 \\ -2k^2 \\ -2k^2 - U_6 \end{bmatrix}}$$

Solving above matrix we get,

$U_1 = 0.1389$

$U_2 = 0.2222$

$U_3 = 0.2500$

$U_4 = 0.2222$

$U_5 = 0.1389$

→ BVP with Neumann BC.

- cooling fin

fin model eqn :

$$\frac{d^2\theta}{d\varepsilon^2} = H^2\theta \qquad \varepsilon \in [0,1]$$

$$M = 4$$

$$\theta(\varepsilon = 0) = 1 \qquad H = 4.$$

$$\left.\frac{d\theta}{d\varepsilon}\right|_{\varepsilon=1} = 0 \qquad \text{center difference.}$$

0 — 0.25 — 0.5 — 0.75 — 1

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$k = \frac{\xi_N - \xi_0}{4}$

$k = 0.25$

$$\frac{-2\theta_m + \theta_{m+1} + \theta_{m-1}}{k^2} = H^2\theta_m$$

$$-2\theta_m + \theta_{m+1} + \theta_{m-1} = H^2\theta_m k^2$$

$$\theta_{m-1} + \theta_m(-2 - H^2k^2) + \theta_{m+1} = 0$$

$$\therefore \theta_{m-1} + \theta_m(-3) + \theta_{m+1} = 0$$

$$[1, -3, 1] \quad ; \quad m \in 1, 2, 3$$

$$\begin{bmatrix} -3 & 1 & 0 \\ 1 & -3 & 1 \\ 0 & 1 & -3 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}$$

$$\frac{\theta_{m+1} - \theta_{m-1}}{2k} = \frac{d\theta}{d\xi}\Big|_{x = x_m}$$

$m \in 1, \dots, 3$

$$\frac{\theta_4 - \theta_3}{0.5} =$$

$$\begin{bmatrix} -3 & 1 & 0 \\ 1 & -3 & 1 \\ 0 & 1 & -3 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ -\theta_4 \end{bmatrix}$$

$-3\theta_1 + \theta_2 = -1$ | $\frac{\theta_5 - \theta_3}{0.5} = 0$

$\theta_1 - 3\theta_2 + \theta_3 = 0$ | $\theta_5 = \theta_3$

[Ghost point method] $\theta_2 - 3\theta_3 = -\theta_4$

for $m = 4 \Rightarrow \theta_3 - 3\theta_4 + \theta_5 = 0$

$\xi_5 \rightarrow$ fictitious node [note: BD not used bcoz it is 1st order accurate]

$\theta_1 - 3\theta_2 + \theta_3 = 0$

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$\theta_2 - 3\theta_3 + \theta_4 = 0 \longrightarrow -1 + 3\theta_1 - 3\theta_3 + \frac{2\theta_3}{3} = 0$

$2\theta_3 - 3\theta_4 = 0$

$\theta_2 = -1 + 3\theta_1$

$\theta_1 - 3(-1 + 3\theta_1) + \theta_3 = 0$

$\theta_1 + 3 - 9\theta_1 + \theta_3 = 0$

$-8\theta_1 + \theta_3 = -3$

$3\theta_1 - \frac{7\theta_3}{3} = 1$

$\therefore \theta_1 = 0.3829787$

$\theta_3 = 0.06382979$

$\theta_2 = -1 + 3\theta_1$

$= 0.1489861$

$\theta_4 = \frac{2\theta_3}{3}$

$\theta_4 = 0.04255319$

$\therefore \theta_1 = 0.3830$

$\theta_2 = 0.1489$

$\theta_3 = 0.0638$

$\theta_4 = 0.0425$

Analytical sol^n

$$\frac{d^2\theta}{d\xi^2} = H^2\theta$$

$$D^2 - H^2\theta = 0$$

$$\theta = A\sinh 4\xi + B\cosh 4\xi$$

$$\boxed{1 = B}$$

$$\frac{d\theta}{d\xi} = 4A\cosh 4\xi - B \times 4 \times \sinh 4\xi$$

$$0 = 4A \times \cosh 4 - 4\sinh 4$$

$$\cancel{4}\sinh 4 = \cancel{4}A\cosh 4$$

$$\boxed{A = 1.1578213}$$

$$\theta = 1.1578213 \sin(4\xi) + \cos(4\xi)$$

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$$\frac{d^2\theta}{d\xi^2} = H^2\theta = 16\theta$$

$$\theta = Ae^{4\xi} + Be^{-4\xi}$$

$\therefore\ 1 = Ae^{0} + Be^{0}$ - - - (1). $A + B = 1$

$$\frac{d\theta}{d\xi} = 4Ae^{4\xi} - 4Be^{-4\xi}$$

$$0 = 4Ae^{4} - 4Be^{-4}$$

$0 = Ae^{4} - Be^{-4}$ - - (2) $Ae^{4} - Be^{-4} = 0$

$$A = 0.0003354$$
$$B = 0.9996646$$

$$\therefore\ \boxed{\theta = 0.0003354\, e^{4\xi} + 0.9996646\, e^{-4\xi}}$$

ξ	θ_N	θ_A
0	1	1
0.25	0.3829	0.3686678
0.5	0.1489	0.1377682
0.75	0.0688	0.0565071
1.00	0.0426	0.0366217

→ Remarks:

1. Ghost point method. @: ficticious node
2. CD(system) + BD(BC) - but there is inconsiste inaccuracy
3. to avoid concern in 1 & 2 we use 3 point FDM
4. Mesh refinement. (Δx)

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→ Mesh refinement:

old grid: $\xi=0$ … $\xi=1$; 0, 0.25, 0.5, 0.75, 1 — 5 grid points

new grid: 0 … 1 — 9 grid points

new grid pts = 2×(old grid points) − 1

m=1 $\quad -2.25\theta_1 + \theta_2 = -1$

m=2 $\quad \theta_1 - 2.25\theta_2 + \theta_3 = 0$

m=3 $\quad \theta_2 - 2.25\theta_3 + \theta_4 = 0$

m=4 $\quad \theta_3 - 2.25\theta_4 + \theta_5 = 0$

m=5 $\quad \theta_4 - 2.25\theta_5 + \theta_6 = 0$

m=6 $\quad \theta_5 - 2.25\theta_6 + \theta_7 = 0$

m=7 $\quad \theta_6 - 2.25\theta_7 + \theta_8 = 0$

m=8 $\quad \theta_7 - 2.25\theta_8 + \theta_9 = 0$

$$\frac{\theta_9 - \theta_7}{2(1/8)} = 0$$

$\theta_9 = \theta_7$

$\theta_7 = 0.0429$

$\theta_9 = 0.0429$

$\theta_8 = 0.0381$

$\theta_6 = -\theta_8 + 2.25\times\theta_7$

$\theta_6 = 0.0584$

$\theta_6 = 0.0885$

~~θ_4~~

$\theta_2 = -1 + 2.25\theta_1$

$\theta_1 + 22.5 - 5.0625\theta_1 + \theta_3 = 0$

$-4.0625\theta_1 + \theta_3 = 2.25$

$-1 + 2.25\theta_1 - 2.25\theta_3$

$+\left(\frac{\theta_3 + \theta_5}{2.25}\right) = 0$

$2.25\theta_1 - 1.805\theta_3$

$= 0.9607$

	ξ	θ_A	$\theta_N(M=4)$	$\theta_N(M=8)$
θ_0	0	1	1	
θ_1	0.125	0.6069		1
θ_2	0.25	0.3687		0.61
θ_3	0.375	0.2246	0.8829	0.3725
θ_4	0.5	0.1378		0.2281
θ_5	0.625	0.0861	0.1489	0.1407
θ_6	0.75	0.0565		0.0885
θ_7	0.825	0.0460	0.0638	0.0584
θ_8	1	0.0366		0.0429
			0.0426	0.0381

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→ 3 point FDM

3. $y(x_m+h) = y_{m+1} = y_m + h\frac{dy}{dx}\Big|_{x=x_m} + \frac{h^2}{2!}\frac{d^2y}{dx^2}\Big|_{x=x_m} + O(h^3)$

$y(x_m+2h) \quad y_{m+2} = y_m + 2h\frac{dy}{dx}\Big|_{x=x_m} + \frac{(2h)^2}{2!}\, d^2y/dx^2\Big|_{x=x_m} + O(h^3)$

$\boxed{y_{m+2} - 4y_{m+1}}$

$= (y_m - 4y_m) + \frac{dy}{dx}\Big|_{x=x_m}(2h-4h) + \frac{d^2y}{dx^2}(2h^2-2h^2) + O(h^3)$

$y_{m+2} - 4y_{m+1} = -3y_m - 2h\frac{dy}{dx}\Big|_{x=x_m} + O(h^3)$

$\frac{4y_{m+1} - y_{m+2} - 3y_m}{2h} + O(h^2) = \frac{dy}{dx}\Big|_{x=x_m}$

$\frac{dy}{dx}\Big|_{x=x_m} = \frac{-3y_m + 4y_{m+1} - y_{m+2}}{2h} + O(h^2)$

--- 2nd order accurate.
--- 3 point f o.

$\boxed{y_{m-2} - 4y_{m-1}} = ?$

$y_{m-1} = y(x_m - h) = y_m - h\frac{dy}{dx}\Big|_{x=x_m} + \frac{h^2}{2!}y''_m + O(h^3)$

$y_{m-2} = y(x_m-2h) = y_m - 2hy'_m + 2h^2y''_m + O($

$y_{m-2} - 4y_{m-1}$
$= (y_m - 4y_m) + y'_m(-2h+4h) + 0 + O(h^3)$

$\frac{y_{m-2} - 4y_{m-1} - y_m + 4y_m}{2h} + O(h^2) = y'_m$

$y'_m = \frac{y_{m-2} - 4y_{m-1} + 3y_m}{2h} + O(h^2)$

--- 3 point BD

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ϕ (Prev)	θ_N	with 3 point BD
θ_0	1	
θ_1	0.3824	
θ_2	0.1471	
θ_3	0.0588	
θ_4	0.0294	

$$-3\theta_1+\theta_2=-1 \rightarrow \theta_1=\frac{+1}{3}+\frac{\theta_2}{3}$$

$$\theta_1-3\theta_2+\theta_3=0 \rightarrow \frac{1}{3}+\frac{\theta_2}{3}-3\theta_2+\theta_3=0$$

$$\theta_2-3\theta_3+\theta_4=0$$

$$0=\frac{\theta_2-4\theta_3+3\theta_4}{2\times 1/4} \qquad -\frac{8}{3}\theta_2+\theta_3=-1/3$$

$$\theta_2-4\theta_3+3\theta_4=0$$

$$\theta_2-3\theta_3+\theta_4=0$$

$$-\frac{8}{3}\theta_2+\theta_3+0\theta_4=-1/3$$

$\therefore$

$\theta_2=0.1471$	$\theta_1=0.3824$
$\theta_3=0.0588$	
$\theta_4=0.0294$	

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→ BVP with Robin BC

$$p(x)\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x) \quad \text{---- system}$$

$$x \in [a, b]$$

$a_0 y(a) + b_0 y'(a) = C_0$ — 3 pt FD

$a_1 y(b) + b_1 y'(b) = C_1$ — 3 pt BD

S1: $k = \frac{b-a}{M}$

S2: ~~$p(x) \times$~~ [Discretize ODE

$$[2P_m - q_m k]\, y_{m-1} + [-4P_m]\, y_m + [2P_m + q_m k]\, y_{m+1} = r_m \times 2k^2 \quad \text{--- (1)}$$

$$m \in 1, 2, 3, \ldots, M-1$$

$$y'_m = \frac{-3y_m + 4y_{m+1} - y_{m+2}}{2k}$$

$$y'(a) = \frac{-3y(a) + 4y_1 - y_2}{2k} \quad \text{--- 3 pt FD}$$

$$2ka_0 y_0 - 3b_0 y_0 + 4b_0 y_1 - b_0 y_2 = 2kC_0$$

$$y_0(2ka_0 - 3b_0) + 4b_0 y_1 - b_0 y_2 = 2kC_0 \quad \text{--- (2)}$$

$$y'_m = \frac{y_{m-2} - 4y_{m-1} + 3y_m}{2k}$$

$$y'(b) = y'_M = \frac{y_{M-2} - 4y_{M-1} + 3y_M}{2k}$$

$$2ka_1 y_M + b_1 y_{M-2} - b_1 4 y_{M-1} + 3b_1 y_M = C_1 2k$$

$$b_1 y_{M-2} - 4b_1 y_{M-1} + y_M(3b_1 + 2ka_1) = 2kC_1 \quad \text{--- (3)}$$

$$\begin{bmatrix} (3r_0^2 + 3b_0) & b_0' - b_0 & 0 \cdots & 0 \\ -4P_m & 2r_m+2r_m k & 0\ 0 \cdots & 0 \end{bmatrix}_{M+1 \times M+1} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{M-1} \\ y_M \end{bmatrix}_{M+1\times 1} = \begin{bmatrix} 2kc_0 \\ r_0 \times 2k^2 \\ \\ \\ \\ \end{bmatrix}_{M+1\times 1}$$

$$\begin{bmatrix} (2kc_0 - 3b_0) & 4b_0 & -b_0 & 0\ 0 \cdots & 0 \\ 2r_m - 2r_m k & -4P_m & 2r_m+2r_m k & 0\ 0 \cdots & 0 \\ 0 & 2r_2 - 2r_2 k & -4P_2 & 2r_m+2r_m k & 0 \cdots 0 \\ \\ 0\ 0\ 0 \cdots & 0 & b_1 & -4b_1 & 3b_1+2kc_1 \end{bmatrix}_{M+1 \times M+1} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix}_{M+1\times 1} = \begin{bmatrix} 2kc_0 \\ 2k^2 r_1 \\ 2k^2 r_2 \\ \\ 2kc_1 \end{bmatrix}_{M+1\times 1}$$

→ Shooting method : $\boxed{BVP}$

ODE (2nd or higher order) ⇒ Convert to a set of first order ODE (IVP)

BCs

pb :-

$$\frac{d^2y}{dx^2} = f\left(x, y, \frac{dy}{dx}\right) \quad \text{--- ODE}$$

$$\left.\begin{aligned} y(x=0) &= \alpha \\ y(x=a) &= \beta \end{aligned}\right\} BC$$

$\cancel{dy/dx} = \theta_1$

$\cancel{\frac{d\theta_1}{dx} = f(x, y, \theta_1)}$

$\cancel{\frac{d\theta_1}{dx} = \theta_2}$

$\cancel{\theta_2 = f(x, \theta)}$

IVP

$y = y_1$

$\frac{dy_1}{dx} = y_2$

$\frac{dy_2}{dx} = f(x, y_1, y_2)$

$y_1(x=0) = \alpha$

$y_2(x=0) = r$ (assumed)

Step-2:

$y_1(x=h),\ y_1(x=2h),\ y_1(3h)\ ---\ y_1(x=a)$

$y_2(x=h),\ y_2(2h),\ y_2(3h)\ ---\ y_2(x=a)$

Step-3:

$$|y_1(a)-\beta| \le tol$$

reassume $y_2(x=0)$??

Remarks: ① Linear interpolation to assume $y_2(0)$.

② It is analogus to a procedure of firing object at stationary target.

example: $\dfrac{d^2y}{dx^2} = 5y + 10x(1-x)$

$y = y_1$	$y(0)=0$
$\dfrac{dy_1}{dx} = y_2$ --- ①	$y(9)=0$
$\dfrac{dy_2}{dx} = 5y_1 + 10x(1-x)$ -- ②	$M=3$
	$tol = 10^{-6}$.
~~y_2~~ Explicit Euler,	$k = \dfrac{9-0}{3}$
$y_2^{(k+1)} = y_2^k + h(5y_1^k + 10x(1-x))$	$k=h=3$

$x_0=0$, $x_1=3$, $x_2=6$, $x_3=9$

$y_2(3) = y_2(0) + 3\times(5\times0 + 10\times0)$

$y_2(3) = 4.$

y_2^0(assumed)

$y_1^{k+1} = y_1^k + h\, y_2^k$

$y_1(3) = 0 + 3\times(4)$

$y_1(3) = 12$

$y_2^{(6)} = y_2(3) + 3\times(5y_1(3) + 10\times 3\times -2)$

$y_2^{(6)} = 4 + 3\times(5\times 12 - 60)$

$y_2^{(6)} = 4.$

$y_1^{(6)} = y_1(3) + h\,y_2(3)$

$= 12 + 3\times 4$

$y_1^{(6)} = 24.$

$y_2^{(9)} = (5y_1(6) + 10\times 6\times -5)\times 3 + y_2(6).$

$= 4 + 3\times(5\times 24 - 300)$

$y_2^{(9)} = -536.$

$y_1^{(9)} = y_1(6) + 3\,y_2(6)$

$= 24 + 3\times 4$

$y_1^{(9)} = 24 + 12 = 36.$

$\therefore$ ~~tot~~ $|36 - 0|$ is not less than tolerance.

$y_2(0) = -2$ (new assumed.)

$y_1^{(k+1)} = y_1^{(k)} + h\,y_2^{(k)}$

$y_2^{(k+1)} = y_2^{(k)} + h(5y_1^{(k)} + 10x^k(1 - x^k))$

$\cancel{y_2^{(k+1)}}$

$y_{11} = y_{10} + 3\times y_{20}$

$= 0 + 3\times -2$

$y_{10} = 0$ $\quad \boxed{y_{11} = -6}$

$y_{21} = y_{20} + 3(5y_{10} + 10\times 0)$

$y_{21} = -2 + 15\times 0 = -2$

$y_{21} = -2.$

$y_{12} = y_{11} + 3\times y_{21} = -6 + 3\times -2$

$y_{12} = -12$

$y_{22} = -2 + 3\times(5\times -6 \cdot 3 + 10\times 3\times -2)$

$y_{22} = -272.$

$y_{13} = y_{12} + 3 \times y_{28}$

$y_{13} = -12 + 3 \times -272$

$= \cancel{-12-6} \quad -828$

$\cancel{= -18}$

$|y_{18} - 0| \simeq \leq tol$

Interpolating

$4 \longrightarrow 36$

$q \quad 0$

$-2 \quad -828$

$$\frac{-828-36}{-2-4} = \frac{0-36}{q-4}$$

$q = 3.75$

$y_2(0) = 3.75$

$y_{11} = y_{10} + h y_{20}$

$= 0 + 3 \times 3.75$

$\boxed{y_{11} = 11.25}$

$y_{21} = y_{20} + h(5y_{10} + 10x_0(1-x_0))$

$= 3.75$

$y_{12} = y_{11} + 3 \times y_{21}$

$= 22.5$

$y_{22} = y_{21} + h(5y_{12} + 10x_1(1-x_1))$

$y_{22} = 161.25$

$y_{13} = y_{12} + 3 \times y_{22}$

$|y_{13} - 0| = 0 \leq tol$

~~tol~~

Non-linear BVP.

$$\frac{d^2y}{dx^2} + y^2\frac{dy}{dx} = 0 \qquad y(0)=1 \qquad x \in [0,4]$$
$$y(4)=0.2$$
$$M=4$$

$k=1$

$x_0=0,\ x_1=1,\ x_2=2,\ x_3=3,\ x_4=4.$

$$\frac{y_{m+1}+y_{m-1}-2y_m}{k^2} + \cancel{2}\times\left(\frac{y_m y_{m+1} - y_m y_{m-1}}{2k}\right) = 0$$

$$y_{m+1} + y_{m-1} - 2y_m + y_m k y_{m+1} - y_m k y_{m-1} = 0$$

$$\cancel{\boxed{y_{m-1}(1-k) - 2y_m + y\,y_{m+1}(k+1) = 0}}$$

$$\cancel{-2y_m + 2y_{m+1} = 0}$$
$$\cancel{y_m + y_{m+1} = 0}$$
$$\cancel{m \in 1,2,3}$$

$$\cancel{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix}}$$

$$y_{m+1} + y_{m-1} - 2y_m + k y_m y_{m+1} - k y_m y_{m-1} = 0$$

$$y_{m-1}(1-ky_m) - 2y_m + y_{m+1}(1+ky_m) = 0$$

$m \in 1,2,3.$ $\qquad y_0 = 1$

$$y_0(1-y_1) - 2y_1 + y_2(1+y_1) = 0 \qquad y_4 = 0.2$$
$$1 - y_1 - 2y_1 + y_2 + y_2 y_1 = 0$$
$$1 - 3y_1 + y_2 + y_1 y_2 = 0 \quad \text{--- (1).}$$
$$y_1 \times (1-y_2) - 2y_2 + y_3(1+y_2) = 0$$
$$y_1 - y_1 y_2 - 2y_2 + y_3 + y_2 y_3 = 0 \quad \text{--- (2)}$$

$n = 3$

$$0.2(1+y_3) - 2y_3 + y_2(1-y_3) = 0$$

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NR:

$$\therefore Y^{k+1} = Y^k - J_H^{-1} \times G^k$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}^{k+1} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}^k - J_H^{-1} \times \begin{bmatrix} g_1 \\ g_2 \\ g_3 \end{bmatrix}^k$$

$$J_H = \begin{bmatrix} \frac{\partial g_1}{\partial y_1} & \frac{\partial g_1}{\partial y_2} & \frac{\partial g_1}{\partial y_3} \\ \frac{\partial g_2}{\partial y_1} & \frac{\partial g_2}{\partial y_2} & \frac{\partial g_2}{\partial y_3} \\ \frac{\partial g_3}{\partial y_1} & \frac{\partial g_3}{\partial y_2} & \frac{\partial g_3}{\partial y_3} \end{bmatrix}$$

$$\boxed{Y^{k+1} = Y^k - J_k^{-1} F_k}$$

$$J_k^{-1} = \begin{bmatrix} -3+y_2^k & 1+y_1^k & 0 \\ 1-y_2^k & -2+y_3^k-y_1^k & 1+y_2^k \\ 0 & 1-y_3^k & -1.8-y_2^k \end{bmatrix}^{-1}$$

$$F_k = \begin{bmatrix} 1-3y_1+y_2+y_1y_2 \\ y_1-2y_2+y_3+y_2y_3-y_2y_1 \\ 0.2+y_2-1.8y_3-y_3y_2 \end{bmatrix}^k$$

$$Y^1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad Y^2 = \begin{bmatrix} 0.466667 \\ 0.4 \\ 0.38333 \end{bmatrix}$$

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$$Y^3 = \begin{bmatrix} 0.49932 \\ 0.830612 \\ 0.251701 \end{bmatrix}$$

$$Y^4 = \begin{bmatrix} 0.500001 \\ 0.833336 \\ 0.249999 \end{bmatrix}$$

$$Y^5 = \begin{bmatrix} 0.5 \\ 0.838883 \\ 0.25 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.838333 \\ 0.25 \end{bmatrix}$$

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→ Partial Differential equation

its an eqn which consists of 1 ~~or~~ more dependent variable wrt more than 1 independent variable.

$$\cancel{A\frac{\partial^2 y}{\partial x^2} + B\frac{\partial^2 y}{\partial x \partial y} + C\frac{\partial^2 y}{\partial y^2} + E\frac{\partial y}{\partial t} + Fy = G}$$

Reference eq.

$$\boxed{A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + Fu = G}$$

$A, B, C, D, E, F, G \Rightarrow$ coefficients

$$AU_{xx} + BU_{xy} + CU_{yy} + DU_x + EU_y + FU = G$$

ODE	PDE
1. Independent variable	1. >1 independent variable
2. IVP: IC BVP: BC	2. Boundary conditions or IC + BC [Initial Boundary value Problem
3.	3. Calculate at different nodes
4. Solution plot looks like a curve	4. Solution plot looks like a surface.

- $$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2}$$

IC at $t = 0$
BC at $x = a$
$x = b$

Numerical methods:

1. FDM
2. FEM
3. FVM (Finite volume method)

FDM:

→ Leap-frog
→ Method of lines
→ Lax-friedrichs
→ Dufort-Frankel
→ Crank-Nicholson

CD

$$\left(\frac{\partial u}{\partial x}\right)_m = \frac{U_{m+1} - U_{m-1}}{2k} + O(k^2)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_m = \frac{U_{m-1} - 2U_m + U_{m+1}}{k^2} + O(k^2)$$

FD

$$\left(\frac{\partial u}{\partial x}\right)_m = \frac{U_{m+1} - U_m}{k} + O(k)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_m = \frac{U_{m+2} - 2U_{m+1} + U_m}{k^2} + O(k)$$

BD

$$\left(\frac{\partial u}{\partial x}\right)_m = \frac{U_m - U_{m-1}}{k} + O(k)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_m = \frac{U_m - 2U_{m-1} + U_{m-2}}{k^2} + O(k)$$

Algorithm:

S1: Discretise surface regime into grid of nodes.

S2: Use FDM to discretise PDE.

S3: BC's and IC's to get sol^n.

ex - one-way wave eq^n:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$a>0$ $a = const$

$t \in (0, \infty)$

$x \in (0, 1)$

$$t_n = t_0 + nh$$

$h = \Delta t$

$n \in 0, 1, 2, ---- N$

$$x_m = x_0 + mk$$

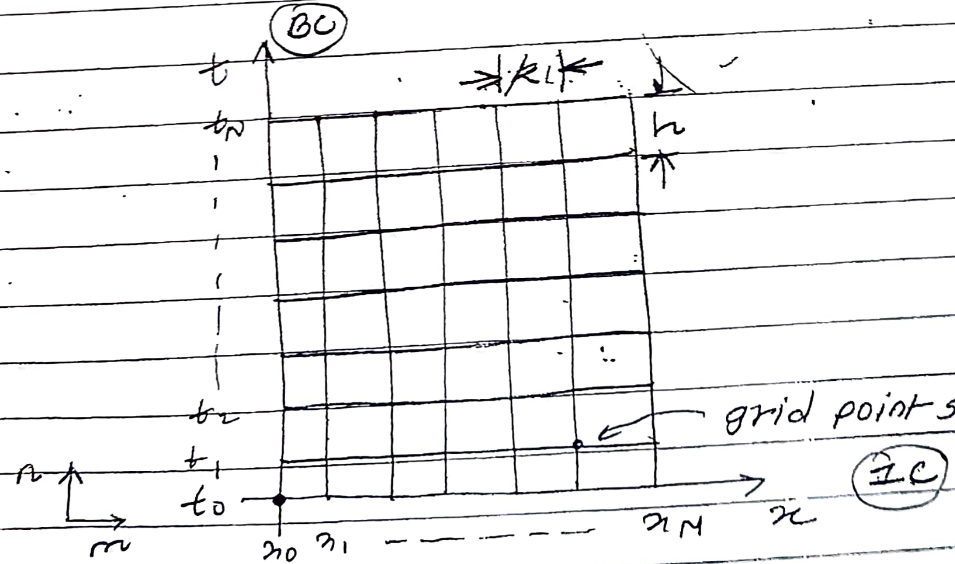
$k = x_M - x_0 / M$

$m \in 0, 1, 2, --- M$

follow: u(space, time)

IC $u(x, 0)$ ~~$= u(0, 0)$~~ $x \in [0, 1]$

BC $u(0, t)$ $t \in [0, \infty)$



→ Forward in time and forward in space (FTFS)

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$$\frac{\partial u}{\partial t} = u_t(x_m, t_n) = \frac{U_{m,n+1} - U_{m,n}}{h} + O(h)$$

---- Forward difference

$$\frac{\partial u}{\partial x} = u_x(x_m, t_n) = \frac{U_{m+1,n} - U_{m,n}}{k} + O(k)$$

---- Forward difference

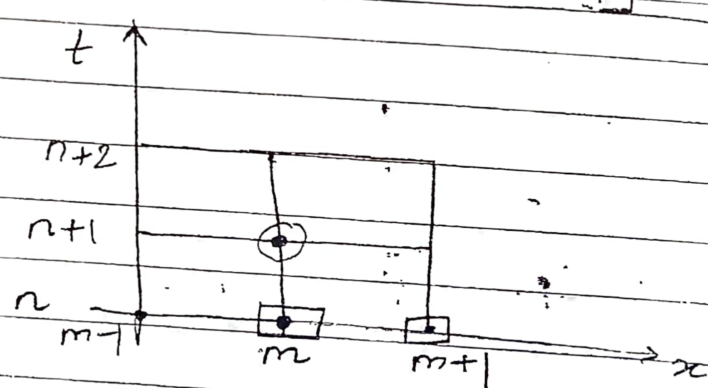
$$\frac{U_{m,n+1} - U_{m,n}}{h} + \frac{a}{k}\left(\frac{U_{m+1,n} - U_{m,n}}{1}\right) = 0$$

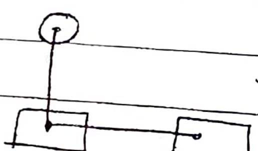
$$+ O(k, h)$$

$$U_{m,n+1} = -\frac{ah}{k}\left(U_{m+1,n} - U_{m,n}\right) + U_{m,n} + \cancel{O(k, k^2)}$$

$$\boxed{U_{m,n+1} = -\frac{ah}{k} U_{m+1,n} + U_{m,n}\left(1 + \frac{ah}{k}\right)}$$

---- FTFS





stencil

O → unknown

□ → known

Remarks:

1. 1st order accurate in both space and time.
2. One-step

Forward in time and backward is space [FTBS

$$\frac{\partial u}{\partial t} = U_t(x_m, t_n) = \frac{U_{m,n+1} - U_{m,n}}{h} + O(h)$$

$$\frac{\partial u}{\partial x} = U_x(x_m, t_n) = \frac{U_{m,n} - U_{m,n}}{k} + O(k)$$

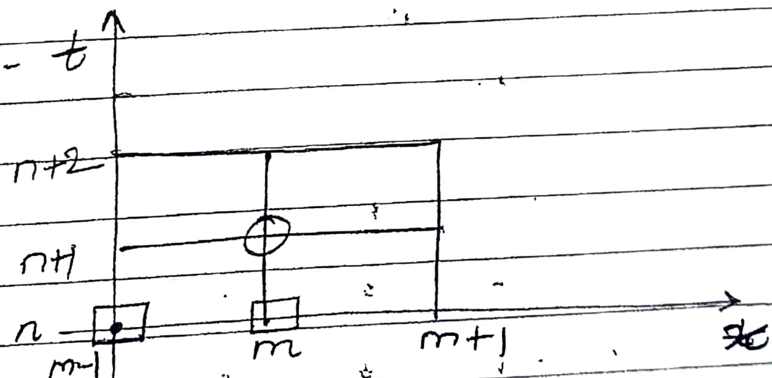
$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$$\frac{U_{m,n+1} - U_{m,n}}{h} + a\left[\frac{U_{m,n} - U_{m-1,n}}{k}\right] + O(h,k) = 0$$

$$U_{m,n+1} = \frac{+ah}{k} U_{m-1,n} + U_{m,n}\left[\frac{-ah}{k} + 1\right].$$

$$\boxed{U_{m,n+1} = U_{m,n}\left(1 - \frac{ah}{k}\right) + \frac{ah}{k} U_{m-1,n} + O(h,k)}$$

graphical representation



$m = 1, 2, \ldots M-1$

stencil:

Remarks:

① 1st order accurate in both space and time

② One-step.

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- Central in time and central in space: [Leap Method]

$$\frac{\partial u}{\partial t} = u_t(x_m, t_n) = \frac{U_{m,n+1} - U_{m,n-1}}{2h} + O(h^2)$$

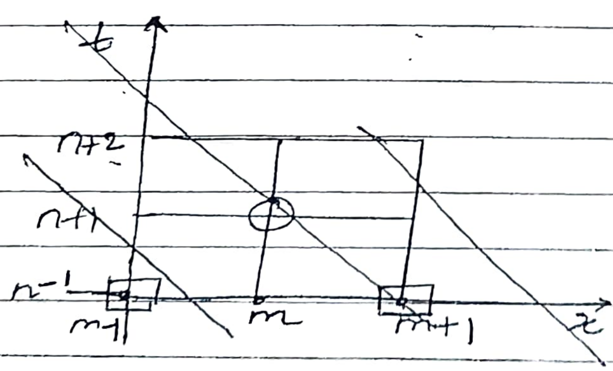
$$\frac{\partial u}{\partial x} = u_x(x_m, t_n) = \frac{U_{m+1,n} - U_{m-1,n}}{2k} + O(k^2)$$

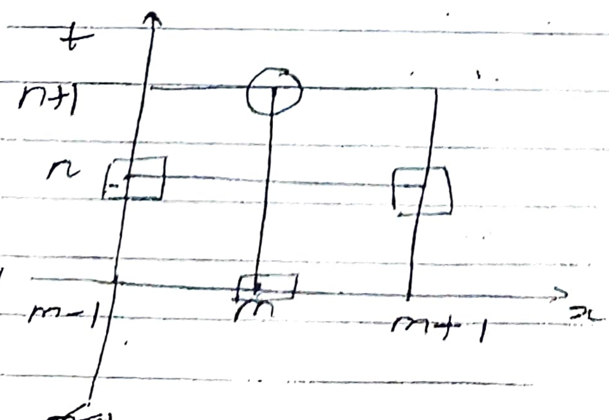
$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

$$\frac{U_{m,n+1} - U_{m,n-1}}{2h} + \frac{a}{2k}\left[U_{m+1,n} - U_{m-1,n}\right] + O(k^2, h^2) = 0$$

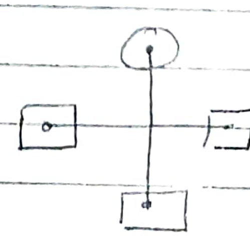
$$U_{m,n+1} = -\frac{a}{2k} \times 2h\left[U_{m+1,n} - U_{m-1,n}\right] + U_{m,n-1} + O(k^2, h^2)$$

$$U_{m,n+1} = -\frac{ah}{k} U_{m+1,n} + \frac{ah}{k} U_{m-1,n} + U_{m,n-1} + O(k^2, h^2)$$





Stencil:



Remarks:

1. Second order accurate in ~~time~~ space & time.
2. ~~one~~ step (information required in n & $n-1$)

→ Method of Lines:

PDE → (ODE) (IVP)

Algorithm:

S-1: Discretise spatial domain $x_0, x_1, \dots, x_M$

$M+1 \Rightarrow$ nodes

S-2: PDE → ODE @ spatial

S-3: Solve the set of ODE's

$\boxed{h = \frac{x_M - x_0}{M}}$

→ Ex

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

[1-Dimensional heat conduction]

$h = 0.025$.

Dirichlet BC's.

$T(0,t) = 0 = T_0(t)$

$T(1,t) = 1 = T_M(t)$

IC;

$T(x,0) = 2$

$x \in (0,1)$

use center difference

$M = 4$

$h = \frac{x_M - x_0}{M}$

S-1: $0 = x_0$ ———— 1 x

S-2: $T_t = \alpha T_{xx}$

$\cancel{\frac{T_{m,n+1} - T_{m,n-1}}{2h} = \alpha}$

$$\frac{dT_m}{dt} = \alpha \left[\frac{y_{m-1,n} - 2y_{m,n} + y_{m+1,n}}{h^2} \right.$$

$y = T$.

$m = 1, 2, \dots, M-1$

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$$\frac{dT_m}{dt} = \alpha \left[\frac{T_{m-1} - 2T_m + T_{m+1}}{k^2} \right]$$

5-3.

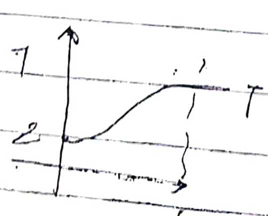
$m=1$ $$\frac{dT_1}{dt} = \frac{\alpha}{k^2}\left[T_0 - 2T_1 + T_2 \right]$$

$m=2$ $$\frac{dT_2}{dt} = \frac{\alpha}{k^2}\left[T_1 - 2T_2 + T_3 \right]$$

$m=M-1$ $$\frac{dT_{M-1}}{dt} = \frac{\alpha}{k^2}\left[T_{M-2} - 2T_{M-1} + T_M \right]$$

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots -2 & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ \vdots \\ T_{M-1} \end{bmatrix} = \begin{bmatrix} \frac{k^2}{\alpha}\frac{dT_1}{dt} - T_0 \\ \vdots \\ \frac{k^2}{\alpha}\frac{dT_{M-1}}{dt} - T_M \end{bmatrix}$$

$$\underset{M-1 \times 1}{\begin{bmatrix} \frac{k^2}{\alpha}\frac{dT_1}{dt} - 0 \\ \frac{k^2}{\alpha}\frac{dT_2}{dt} \\ \vdots \\ \frac{k^2}{\alpha}\frac{dT_{M-1}}{dt} - 1 \end{bmatrix}} = \underset{M-1 \times M-1}{\begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots -2 & 1 \end{bmatrix}} \times \underset{M-1 \times 1}{\begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{M-1} \end{bmatrix}}$$



$\boxed{M = 4}$

$\alpha = 0.00138$

$k = 0.25$

$$\frac{k^2}{\alpha} = 45.28986$$

$\boxed{\text{soln at } 5.5.}$??

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$$\cancel{T_1 = T_0 + h\left(\frac{dT_0}{dt}\right)_{t=t_0}}$$

Using Euler :

$$T_2 = T_1 + h\frac{dT_1}{dt} \Rightarrow 40T_2 - 40T_1$$

$$T_3 = T_2 + h\frac{dT_2}{dt} \Rightarrow 40T_3 - 40T_2$$

$$T_4 = T_3 + h\frac{dT_3}{dt} \Rightarrow 40 - 40T_3$$

$$\frac{h^2}{\alpha} = 45.28986$$

$M=4$

$$\begin{bmatrix} 45.28986 \times [40T_2 - 40T_1] \\ 45.28986 \times [40T_3 - 40T_2] \\ 45.28986 [40 - 40T_3] - 1 \end{bmatrix} = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}$$

$$45.28986 \times 40 = \boxed{1811.5944}$$

$$1811.5944\,T_2 - 1811.5944\,T_1 = -2T_1 + T_2$$

$$1810.5944\,T_2 = 1809.5944\,T_1$$

$$\boxed{1.000558\,T_2 = T_1}$$

$$1811.5944\,T_3 - 1811.5944\,T_2 = T_1 - 2T_2 + T_3$$

$$1811.5944 - 1811.5944\,T_3 - 1 = T_2 - 2T_3$$

$$\boxed{1810.5944 = T_2 + 1809.5944\,T_3}$$

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$0 = T_1 + 1809.5944 T_2 - 1810.5944 T_3$

$T_1 - 1.00055 T_2 + 0 T_3 = 0$

$T_1 + 1809.5944 T_2 - 1810.5944 T_3 = 0$

$0 \times T_1 + T_2 + 1809.5944 T_3 = 1810.5944$

$T_1 = 1.00055$
$T_2 = 0.99999$
$T_3 = 1$

$T_{10}, T_{20}, T_{30} = 2$

Using Backward difference method,

$$T_{mn} = T_{mn-1} + h \frac{dT_{mn}}{dt}$$

$$\frac{T_{mn} - T_{m(n-1)}}{h} = \frac{dT_{mn}}{dt}$$

$$-T_{1n-1} = 0.000552 \left(T_{0n}^{\,0} - 2T_{1n} + T_{2n} \right) + T_{1n}$$

$$-T_{1n-1} = -1.001104 T_{1n} + 0.000552 T_{2n}$$

Similarly

$$-T_{2n-1} = 0.000552 T_{1n} - 1.001104 T_{2n} + 0.000552 T_{3n}$$

$$T_{3n} - T_{3n-1} = 0.000552 \left(T_{2n} - 2T_{3n} + T_{4n} \right)$$

$$T_{3n-1} - 0.000552 = -2.0006552 = 0 + 0.000552 T_{2n} - 1.001104 T_{3n}$$

$$\begin{bmatrix} -T_{1\,n-1} \\ -T_{2\,n-1} \\ \left(-T_{3\,n-1} - 0.00052\right) \end{bmatrix} = \begin{bmatrix} -1.001104 & 0.000552 & 0 \\ 0.000552 & -1.001104 & 0.000552 \\ 0 & 0.000552 & -1.001104 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}$$

$$\downarrow \qquad\qquad \downarrow \qquad\qquad \downarrow$$

$$P_{n-1} \qquad\qquad A \qquad\qquad T_i$$

3x3

$$A P_n = P_{n-1}$$

$$P_n = A^{-1} P_{n-1}$$

iterating we get, at steady state

tolerance $= 10^{-6}$

$T(0) = 0$

$T(0.25) = 0.2531$

$T(0.5) = 0.5044$

$T(0.75) = 0.7531$

$T(1) = 1$

→ Lax-friedrichs method:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

FTCS

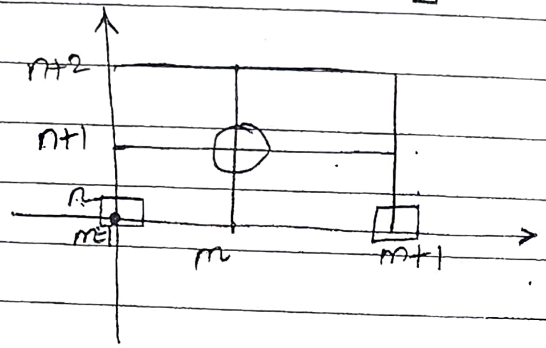
$$\frac{U_{m,n+1} - U_{m,n}}{h} + a\left[\frac{U_{m+1,n} - U_{m-1,n}}{2k}\right] =$$

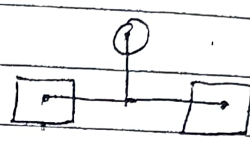
$$\frac{U_{m,n+1} - U_{m,n}}{h} = -a\left[\frac{U_{m+1,n} - U_{m-1,n}}{2k}\right] + O(k$$

$$U_{m,n} = \frac{1}{2}\left(U_{m+1,n} + U_{m-1,n}\right)$$

$$U_{m,n+1} = \frac{-ha}{2k}\left[U_{m+1,n} - U_{m-1,n}\right] + \frac{1}{2}\left(U_{m+1,n} + U_{m-1,n}\right) + O(h, k^2)$$

$$U_{m,n+1} = U_{m+1,n}\left[\frac{1}{2} - \frac{ha}{2k}\right] + U_{m-1,n}\left[\frac{1}{2} + \frac{ha}{2k}\right]$$





Remarks:

→ Unconditionally unstable

→ one step.

→ Bounded soln $\equiv \left|\frac{ah}{k}\right| \leq 1$

- Dufort - frankel

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

CTCS,

$$\frac{U_{m,n+1} - U_{m,n-1}}{2h} = \alpha\left[\frac{U_{m-1,n} - 2U_{m,n} + U_{m+1,n}}{k^2}\right] + O(h^2, k^2)$$

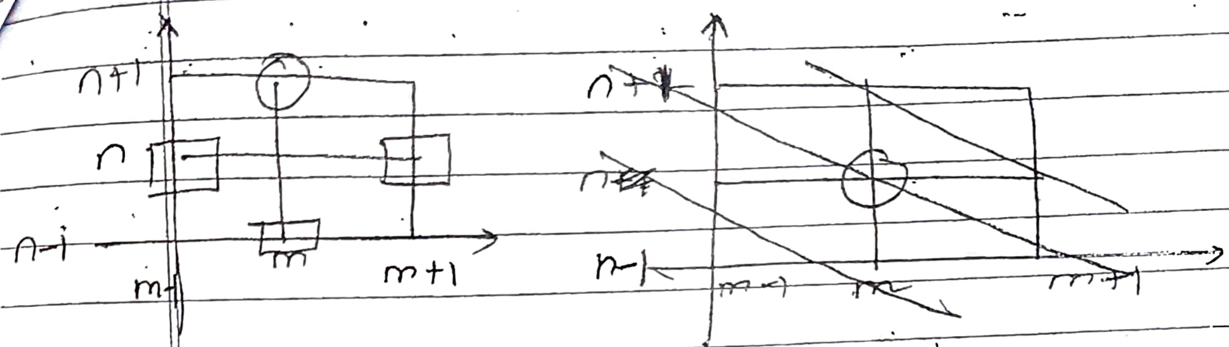
$$U_{m,n} = \frac{1}{2}\left(U_{m,n+1} + U_{m,n-1}\right), \quad \frac{h\alpha}{k^2} = r$$

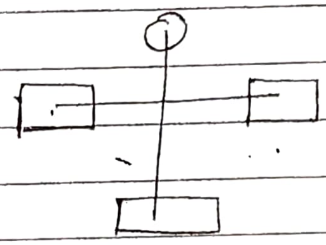
$$U_{m,n+1} = \frac{2h\alpha}{k^2}\left[U_{m-1,n} - \frac{2}{2}\left[U_{m,n+1} + U_{m,n-1}\right] + U_{m+1,n}\right] + U_{m,n-1}$$

$$U_{m,n+1} = 2r\left[U_{m-1,n} - U_{m,n+1} - U_{m,n-1} + U_{m+1,n}\right] + U_{m,n-1}$$

$$U_{m,n+1} = 2r\left[U_{m-1,n} - U_{m,n+1} + U_{m+1,n}\right] + U_{m,n-1}(1-2r)$$

$$U_{m,n+1} = \frac{2r(U_{m-1,n} + U_{m+1,n}) + U_{m,n-1}(1-2r)}{1+2r}$$



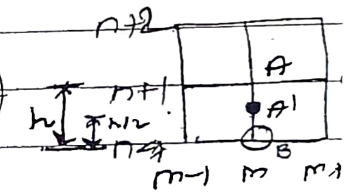


Remarks:

1. Unconditionally stable
2. 2-step method

→ Crank-Nicholson [widely used method]

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad (m, n+1/2)$$



$$U_t(m, n+1/2) = \frac{U_{m,n+1} - U_{m,n}}{\cancel{2}(h/\cancel{2})}$$

$$U_x(m, n+1/2) = \frac{1}{2}\left[U_x(m, n+1) + U_x(m,n)\right]$$

A′ A B

now applying to A′

$$U_x(m, n+1/2) = \frac{1}{2}\left[\frac{U_{m+1,n+1} - U_{m-1,n+1}}{2k} + \frac{U_{m+1,n} - U_{m}}{2k}\right.$$

$\therefore \cancel{U_{m,n+1/2}}$ $\Rightarrow$ ( ) $U_{m-1,n+1}$ + ( ) $U_{m,n+1}$ + ( ) U_{m+}

= ?

maxmind®

$$\frac{U_{m,n+1}-U_{m,n}}{h}+\frac{a}{4k}\left[U_{m+1,n+1}-U_{m-1,n+1}+U_{m+1,n}-U_{m-1,n}\right]=0$$

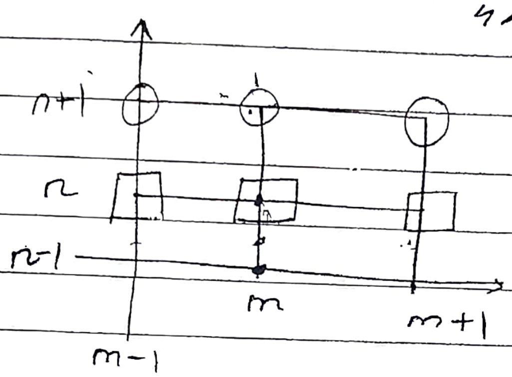
$$-\frac{a}{4k}U_{m-1,n+1}+\frac{1}{h}U_{m,n+1}+\frac{a}{4k}U_{m+1,n+1}$$

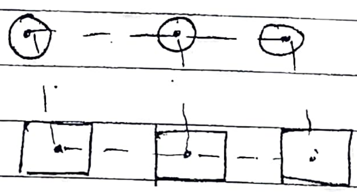
$$+\frac{a}{4k}\left[U_{m+1,n}-U_{m-1,n}\right]$$

$$=0.$$

$$-\frac{ah}{4k}U_{m-1,n+1}+U_{m,n+1}+\frac{ah}{4k}U_{m+1,n+1}$$

$$=-\frac{ah}{4k}\left[U_{m+1,n}-U_{m-1,n}\right]+U_{m,n}$$





Remark:

1. 2nd order accurate in both space and time
2. Implicit [Unconditionally stable]

16

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

BC

$U(0, t) = 0 \rightarrow BC1$

$U(1, t) = 1 \rightarrow BC2$

IC

$U(x, 0) = 2$

$x \in (0, 1)$ & not $[0, 1]$

$$\frac{\partial u}{\partial t} = U_t(m, n+1/2) = \frac{U_{m, n+1} - U_{m, n}}{h}$$

$$\frac{\partial^2 u}{\partial x^2} = U_{xx}(m, n+1/2) = \frac{1}{2}\left(U_{xx}(m, n+1) + U_{xx}(m, n)\right)$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{2}\left[\frac{U_{m-1, n+1} - 2U_{m, n+1} + U_{m+1, n+1}}{k^2} + \frac{U_{m-1, n} - 2U_{m, n} + U_{m+1, n}}{k^2}\right]$$

$$r = \frac{\alpha h}{k^2}.$$

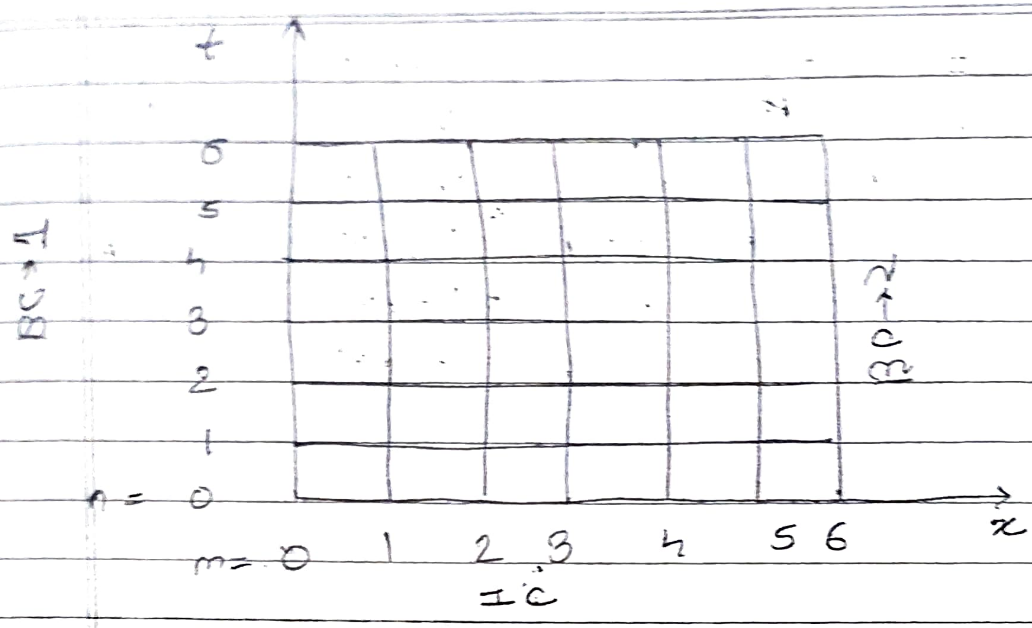
$$\frac{(U_{m, n+1} - U_{m, n})}{1} = \frac{\alpha h}{2k^2}\left[U_{m-1, n+1} - 2U_{m, n+1} + U_{m+1, n+1} + U_{m-1, n} - 2U_{m, n} + U_{m+1, n}\right]$$

$$U_{m, n+1} - \frac{r}{2}U_{m-1, n+1} + r U_{m, n+1} - \frac{r}{2}U_{m+1, n+1}$$

$$= U_{m, n} + \frac{r}{2}\left[U_{m-1, n} - 2U_{m, n} + U_{m+1, n}\right]$$

$$-\frac{r}{2}U_{m-1, n+1} + (1 + r)U_{m, n+1} - \frac{r}{2}U_{m+1, n+1}$$

$$= U_{m, n} + \frac{r}{2}\left[U_{m-1, n} - 2U_{m, n} + U_{m+1, n}\right]$$



M = 6
N = 6

Knowns: U_{10} U_{20} U_{30} U_{40} U_{50} (IC).

m → space, n → time

U_{00} U_{01} U_{02} U_{03} U_{04} U_{05} U_{06} (BC1)

U_{60} U_{61} U_{62} U_{63} U_{64} U_{65} U_{66} (BC2)

$m = 1, 2, 3, \ldots M-1$

$$-\frac{r}{2} U_{m-1,n+1} + (1+r) U_{m,n+1} - \frac{r}{2} U_{m+1,n+1}$$

$$= U_{m,n}(1-r) + \frac{r}{2} U_{m-1,n} + \frac{r}{2} U_{m+1,n} \text{ (completely known)}$$

Note: If $U(x,0) = 2$ at $x \in [0,1]$

then $U_{00} = \dfrac{U(0,t) + U(x,0)}{2}$

$U_{60} = \dfrac{U(6,t) + U(6,0)}{2}$

needs to be considered in IC,

$m = 1$

$$\cancel{r U_{0,n+1}} - (2+2r) U_{1,n+1} + r U_{2,n+1} = b_1$$

$$a_{11} U_{1,n+1} + a_{12} U_{2,n+1} = b_1$$

$m = 2$

$$r U_{1,n+1} - (2+2r) U_{2,n+1} + r U_{3,n+1} = b_2$$

$$a_{21} U_{1,n+1} - \cancel{(2+2r)}\, a_{22} U_{2,n+1} + a_{23} U_{3,n+1} = b_2$$

$$
\begin{array}{c}
\\ \\ m=1 \\ m=2 \\ m=3 \\ m=4 \\ m=5 \\ \cancel{m=6}
\end{array}
\begin{bmatrix}
\overset{-(2+2r)}{a_{11}} & \overset{r}{a_{12}} & 0 & 0 & 0 & 0 \\
0 & \cancel{-(2+2r)} & -(2+2r) & r & 0 & 0 \\
0 & 0 & r & -(2+2r) & r & 0 \\
0 & 0 & 0 & r & -(2+2r) & r \\
0 & 0 & 0 & 0 & r & -(2+2r) \\
0 & 0 & 0 & 0 & 0 & r \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}_{5\times 5}
\begin{bmatrix}
U_{1,n+1} \\ U_{2,n+1} \\ U_{3,n+1} \\ U_{4,n+1} \\ U_{5,n+1} \\ \cancel{U_{6,n+1}}
\end{bmatrix}_{5\times 1}
=
\begin{bmatrix}
b_{1n} \\ b_{2n} \\ b_{3n} \\ b_{4n} \\ b_{5n} \\ \cancel{b_{6n}}
\end{bmatrix}_{5\times 1}
$$

$$
\begin{array}{c}
m=1 \\ m=2 \\ m=3 \\ m=4 \\ m=5
\end{array}
\begin{bmatrix}
-(2+2r) & r & 0 & 0 & 0 \\
r & -(2+2r) & r & 0 & 0 \\
0 & r & -(2+2r) & r & 0 \\
0 & 0 & r & -(2+2r) & 0 \\
0 & 0 & 0 & r & -(2+2r)
\end{bmatrix}_{5\times 5}
\times
\begin{bmatrix}
U_{1,n+1} \\ U_{2,n+1} \\ U_{3,n+1} \\ U_{4,n+1} \\ U_{5,n+1}
\end{bmatrix}_{5\times 1}
=
\begin{bmatrix}
b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5
\end{bmatrix}_{5\times 1}
$$

$\Rightarrow$ Thomas algorithm for solving trigonal matrix.

- Generalised implicit method

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

$$u_t(m, n+1/2) = \frac{u_{m,n+1} - u_{m,n}}{h}$$

$$u_{xx}(m, n+1/2) = \theta\, u_{xx}(m,n) + (1-\theta)\, u_{xx}(m, n+1)$$

$$u_{xx}(m, n+1/2) = \cancel{\theta\, u_{m,n+1} - u_{m,n}} = \theta \left[\frac{u_{m-1,n} - 2u_{m,n} + u_{m+1,n}}{k^2} \right] + (1-\theta) \left[\frac{u_{m-1,n+1} - 2u_{m,n+1} + u_{m+1,n+1}}{k^2} \right]$$

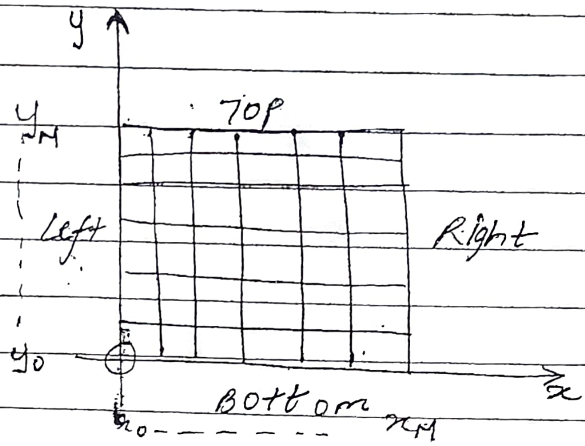
Date ___ Page ___

Elliptic PDE :

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = H(x,y) \quad ---- \quad \left(\begin{array}{l} \text{system eqn} \\ \boxed{\text{Poisson eqn}} \end{array} \right)$$

BC :

$u(x,0) = U_1$ Bottom boundary.



$U(0,y) = U_2$ Left

$U(x,1) = U_3$ Top

$U(1,y) = U_4$ Right

Dirichlet Boundary Condition

Algorithm :

S-1 : Discretise the spatial domain

$$K_1 = \Delta x = x_{i+1} - x_i$$

$$K_2 = \Delta y = y_{i+1} - y_i$$

S2 : ~~Forward~~ Finite difference method is used to discretise PDE

set of algebraic eqn.

S-3 : Deal with BC $\rightarrow$ AEs (if Dirichlet BC are not given)

S-4 : Solve resulting set of AE's.

Date / /
Page

Unknown ⇒ $(M+1)^2$

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = H(x,y)$$

$$U_{xx} + U_{yy} = H(x,y)$$

$$\cancel{U(m-1,m) - 2U(m,m)}$$

$$\frac{U(i-1,j) - 2U(i,j) + U(i+1,j)}{k_1^2}$$

$$+ \frac{U(i,j-1) - 2U(i,j) + U(i,j+1)}{k_2^2} = H(i,j)$$

$$\boxed{k_1 = k_2}$$

$$U(i-1,j) - 4U(i,j) + U(i+1,j) + U(i,j-1) + U(i,j+1) = k^2 H(i,j)$$

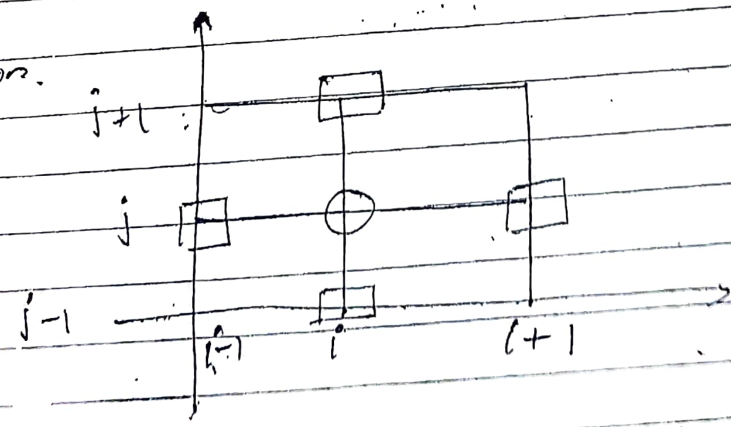
$$U(i,j) = \frac{U(i-1,j) + U(i+1,j) + U(i,j-1) + U(i,j+1) - k^2 H(i,j)}{+4}$$

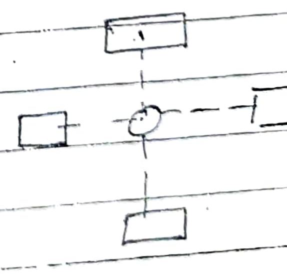
5 point formula,

valid for interior nodes ⇒ $U_{i,j} = \dfrac{U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - k^2 H(i,j)}{4}$ — (

for ⇒ $H = 0$

Graphical representation.





for $H = 0$ [The eqⁿ converts to laplace eqⁿ].

$$1 \le i, j \le M-1$$

no. of eqn from ①

$(M-1)^2$

BC

$U_{i,0} = U_1$ (Bottom) $1 \le i \le M-1$

$U_{0,j} = U_2$ (L) $1 \le j \le M-1$

$U_{i,M} = U_3$ (T) $1 \le i \le M-1$

$U_{M,j} = U_4$ (R) $1 \le j \le M-1$

eqn $\Rightarrow 4(M-1)$

$$U_{00} = \frac{U_1 + U_2}{2}$$

$$U_{0,M} = \frac{U_3 + U_2}{2}$$

$$U_{M,M} = \frac{U_3 + U_4}{2} \qquad \text{Eeqn} = 4.$$

$$U_{M,0} = \frac{U_1 + U_4}{2}$$

$\therefore$ total eqn $= (M-1)^2 + 4(M-1) + 4$

$= (M+1)^2$

Problem :-

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = 0$$

$0 \le x, y \le 1$

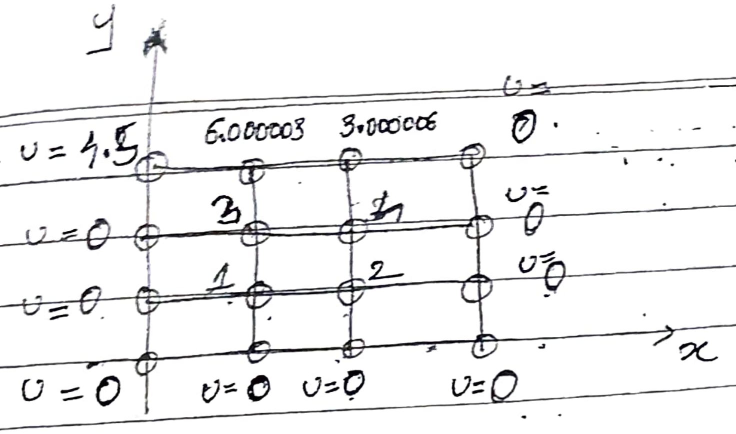
$M = 3$

U_1	B	$U(x,0) = 0$	U_1
U_2	L	$U(0,y) = 0$	U_4
U_3	T	$U(x,1) = x(1-x)$	
U_4	R	$U(1,y) = 0$	

~~$U_{i,j} = U_i$~~

x_0	x_1	x_2	x_M / x_3
0	0.333333	0.666666	1

y_0	y_1	y_2	y_M / y_3
0	0.333333	0.666666	1



1, 2, 3, 4 ⇒ nodes

$$u_{i,j} = \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j+1} + u_{i,j-1}}{4}$$

$$1 \le i,j \le M-1$$

$$u_1 = \frac{1}{4}\left[0 + 0 + u_2 + u_3\right]$$

$$u_2 = \frac{1}{4}\left[u_1 + 0 + 0 + u_4\right]$$

$$u_3 = \frac{1}{4}\left[6 + 0 + u_1 + u_4\right]$$

$$u_4 = \frac{1}{4}\left[3 + u_3 + u_2 + 0\right]$$

$$4u_1 - u_2 - u_3 = 0$$
$$-u_1 + 4u_2 - u_4 = 0$$
$$-u_1 + 4u_3 - u_4 = 6$$
$$-u_2 - u_3 + 4u_4 = 3$$

$$\begin{bmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & +4 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 6 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} \cancel{4} & -1 & 0 & -1 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \end{bmatrix}$$

$$U_1 = \frac{U_2 + U_4}{4}.$$

$$-U_2 - U_4 + 16U_2 - 4U_4 = 0$$

$$15U_2 - 5U_4 = 0$$

$$3\cancel{15}U_2 = \cancel{5}U_4$$

$$U_4 = 3U_2$$

$$-U_2 - U_3 + 12U_2 = 3.$$

$$11U_2 - 3 = U_3$$

$$-U_1 + 44U_2 - 12 - 3U_2 = 0$$

$$-\left(\frac{3U_2 + U_2}{4}\right) + 4\cancel{1}U_2 = 12$$

$\therefore$

$$\boxed{\begin{aligned} U_1 &= 0.625 \\ U_2 &= 0.5 \\ U_3 &= 2 \\ U_4 &= 1.875 \end{aligned}}$$

Pb –

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$

BC

$U = 0$ over the edge $x = 0$

$U = 0$ over the edge $y = 0$

$U = 16 - x^2 - y^2$ at the edge $x + y = 4$

Find U at the nodes of the square ~~with~~ region with mesh lenght 1.

solved in ~~Rough~~ next book

Rough work

Backwa → space

forword → time.

$$\frac{C_{A_{m,n+1}} - C_{A_{m,n}}}{h} + v\left[\frac{C_{A_{m,n}} - C_{A_{m,n-1}}}{k}\right]$$

$$+ k_0 \exp\left[\frac{-\Delta E}{R}\left(\frac{1}{T_{m,n}} - \frac{1}{T_R}\right)\right] = 0$$

$C_{A_{0,n}} = 1$ $\quad T_{0,n} = 500$

$C(A)_{m,n+1}$ $\quad C_{A\,\cancel{m},0} = 1$ $\quad T_{m,0} = 500$

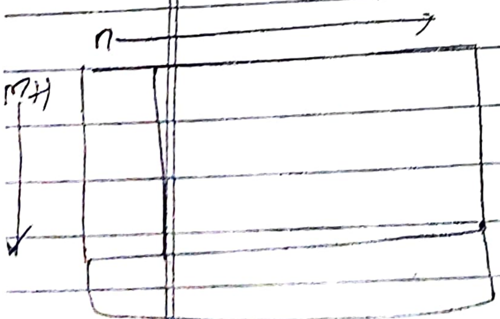
$m+1 \le M$ $\quad k = 0.0025$ $\quad n \in 0, N-1$ $\quad h = 0.001$

$C_{A_{1,n+1}} = f(C_{A_{1,n}} ; C_{A_{0,n}} ; T_{1,n} ; C_{A_{1,n}})$

$C_{A_{1,1}} = f(C_{A_{1,0}} ; C_{A_{0,0}} ; T_{1,0} ; C_{A_{1,0}})$

$C_{A_{2,1}} = f(C_{A_{2,0}} ; C_{A_{1,0}} ; T_{2,0} ; C_{A_{2,0}})$

C_A / 1. / $\quad n = 0.$ $\quad n = 0$



$$\begin{bmatrix} C_{A_{1,1}} \\ \cancel{C_{A_2}} \\ \\ \end{bmatrix} = ($$

$n = 1.$

$T_{A_{1,1}}$

$C_A(2,2)$

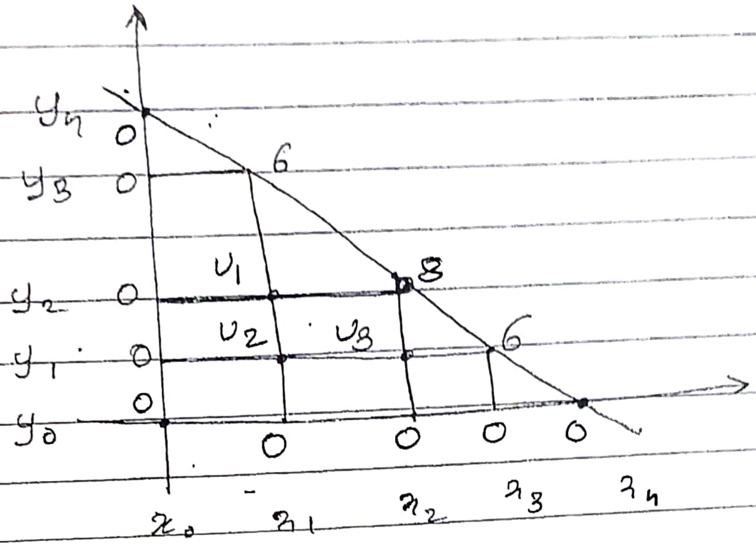
$C_A(1,2)$

$C'A$

$C_{A_{1,2}} = f(C_{A_{1,1}} ; C_{A_{0,1}} , T_{1,1} , C_{A_{1,1}}).$

continue:

16. Graphical representation:



(x, y)	$16-x^2-y^2$
$(1,3)$	6
$(2,2)$	8
$(3,1)$	6

$$u_1 = \frac{1}{4}\left[0+6+8+u_2\right] \quad \text{--- (1)}$$

$$u_2 = \frac{1}{4}\left[u_1+u_3+0+0\right] \quad \text{--- (2)}$$

$$u_3 = \frac{1}{4}\left[8+6+u_2+0\right] \quad \text{--- (3)}$$

from (1), (2) & (3)

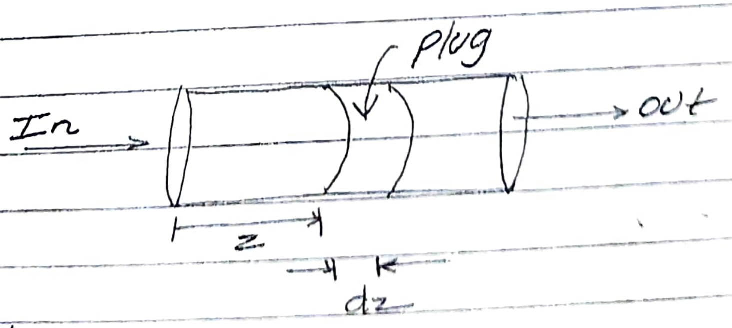
$u_1 = 4$

$u_2 = 2$

$u_3 = 4$

$\Rightarrow$ System with 2 PDE:

PFR:



Assumptions:

1. Perfect mixing (within plug)
2. No variation of conc. of A and Temp. in radial directn

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3. Not heat loss [Adiabatic]

4. Physical properties (ρ, C_p) remain constant

5. Considering 1 directional flow.

6. 2nd order endothermic rxn.

7. Convective velocity is constant

8. ~~axial~~ Diffusion is neglected.

Modelling eqn:

$$\frac{\partial C_A}{\partial t} + v\frac{\partial C_A}{\partial z} + (-r_A) = 0 \quad \text{mass balance}$$

$$\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial t} + \frac{\Delta H(-r_A)}{\rho C_p} = 0 \quad \text{energy balance.}$$

BC's $\quad C_A(0, t) = 1$

$T(0, t) = 500$

IC's $\quad C_A(z, 0) = 1$

$T(z, 0) = 500$

$$-r_A = k C_A^2$$

$$k = k_0 \exp\left[\frac{-\Delta E}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)\right]$$

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Data:

$K_0 = 5$ $\quad h = 0.001$ $\quad$ Use: BSFT Backward in space and forward in time.

$T_r = 500$ $\quad k_1 = 0.08$

$\Delta E = 50 \times 10^3$ $\quad l = 2$ meter

$\Delta H_r = 10 \times 10^3$ $\quad M = 25$.

$v = 0.5$

$\rho C_p = 1000$

$R = 8.314$

Using method of lines we discretise the differential eqn

$$T_{m,n+1} = 0.99375\, T_{m,n} + 0.00625\, T_{m-1,n} - 0.05 \exp\left[\frac{-6013.952869}{T_{m,n}} + 12.027905\right] C_{A_m}^2$$

$n \geq 0$; $m \in [1, M]$

&

$$C_{A_{m,n+1}} = 0.99375\, C_{A_{m,n}} + 0.00625\, C_{A_{m-1,n}} - 0.005 \exp\left[\frac{-6018.952869}{T_{m,n}} + 12.027905\right] C_{A}^2$$

$n \geq 0$; $m \in [1, M]$

know: $C_A(0,n) = 1$ $\quad T(0,n) = 500$

$C_A(m,0) = 1$ $\quad T(m,0) = 500$

first for $m = 1$ $n = 0$.

$C_{A_{1,1}} = f(C_{A_{1,0}} ; C_{A_{0,0}} ; T_{1,0})$ ✓

$m=2$ $C_{A_{2,1}} = f(C_{A_{2,0}} ; C_{A_{1,0}} ; T_{2,0})$ ✓

⋮

$C_{A_{M,1}}$ ✓

then for $m = 1$ $n = 0$.

$T_{1,1} = f(T_{1,0} ; T_{0,0} ; C_{A_{1,0}})$ ✓

$m=2$ $T_{2,1} = f(T_{2,0} ; T_{1,0} ; C_{A_{2,0}})$ ✓

maximind

⋮

$T_{M,1}$ ✓

for $m=1$; $n=1$

$m=1$ $C_{A_{1,2}} = f(C_{A_{1,1}}; C_{A_{0,1}}; T_{1,1})$

$m=2$ $C_{A_{2,2}} = f(C_{A_{2,1}}; C_{A_{1,1}}; T_{2,1})$

$m=M$ $C_{A_{M,2}}$

Same goes for temperature and so on.

S-1: generate function for $C_A(m,n+1)$ & $T(m,n+1)$ computation.

S-2: keeping n same vary m from $1 \rightarrow M$ to find C_A & T at various positions.

S-3: now change n (i.e. go to next time step)
note: after 2st iterations are done start checking tolerance for C_A & T

$$|C_A(m,n+1) - C_A(m,n)| \leq 10^{-6}$$
$$|T(m,n+1) - T(m,n)| \leq 10^{-6}$$

if tolerance condn satisfied then Stop
else

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At 5.5

Z	T		C_A
1.	500		1
2.	496.692		0.6693
3.	494.9565		0.4957
4.	493.9139		0.3914
5.	493.2439		0.3244
6.	492.5358		0.2809
7.	492.3757		0.2536
8.	492.2891		0.2376
9.	492.2462		0.2289
10.	492.2265		0.2246
11.	492.2183		0.2227
12.	492.2151		0.2218
13.	492.2139		0.2215
14.	492.2135		0.2214
15.	492.2134		0.2214
16.	492.2134		0.2213
17.	492.2133		
18.	|		|
19.	|		|
20.	|		|
21.	|		|
22.	|		|
23.	|		|
24.	|		|
25.	|		|
26.	|		0.2213
27.	492.2133		

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Batch Distillation : [for slow process]

If we use continuous distillation for slow process the residence time required is high.

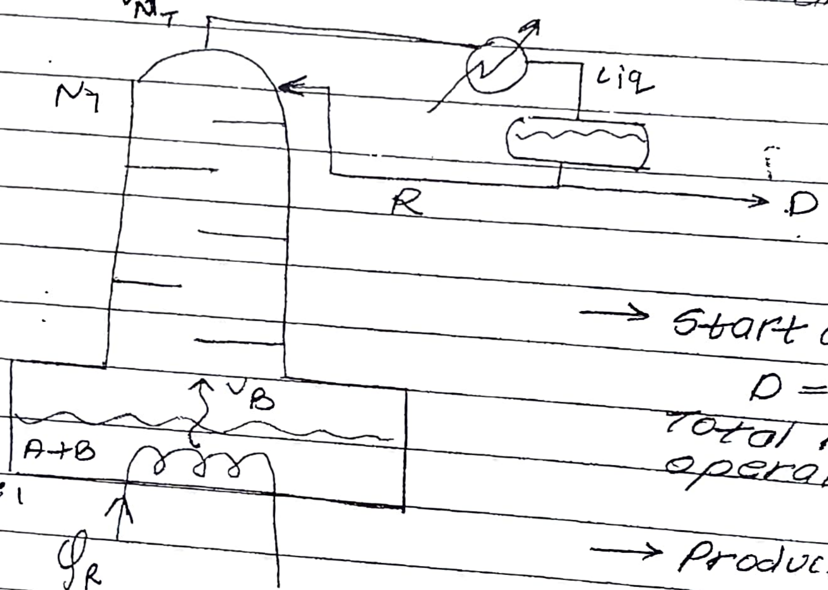
Motivation:

→ To get high value added product.

→ $N_c - 1$ no. of columns for continuous distillation
(N_c → no. of components)

Whereas we can perform same ternary component seperation in batch distillation.

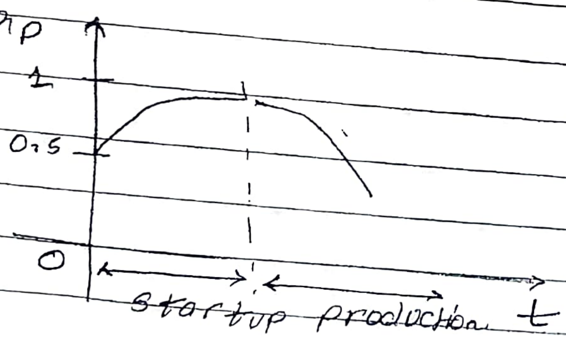
→ ~~Les~~ Less Contamination in batch distillation.



$B = \frac{Q_R}{\lambda_B}$

→ Start up phase:
$D = 0$
Total reflux operation

→ Production phase:
$D \neq 0$
Partial reflux operation



Note: In Batch distillation we are reaching steady state.

Assumptions:

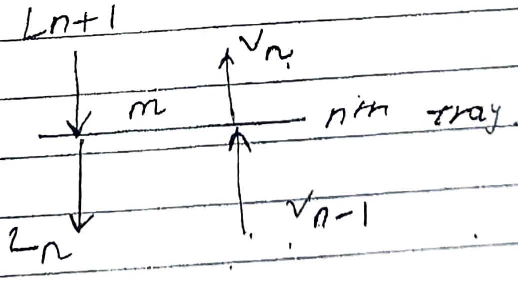
1. Perfect mixing on the trays. [and eq^n]
2. No heat loss (insulated column)
3. P is constant
4. Tray efficiency is fixed η [in practice $\eta \Rightarrow 40-50\%$]

$$\eta = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}} \quad \text{--- Murphy tray efficiency}$$

↳ eq^m ~~compo~~ vapour composition

$\therefore y_n = ??$

5. No vapour hold up [negligible]
6. Liquid hold up is variable
7. Liquid phase is non-ideal but vapour phase is considered ideal.



Will give { modelling

$m \Leftarrow$ total $\Rightarrow$ $L_{n+1} + V_{n-1} - V_n - L_n = \frac{dm_n}{dt}$

$x \Leftarrow$ Component $\Rightarrow$ $x_{n+1} L_{n+1} + y_{n-1} V_{n-1} - x_n L_n - y_n V_n = \frac{d\, x_n m_n}{dt}$

V (vapour flow rate) $\Leftarrow$ energy balance,

$L_{n+1} C_{P_L} T_{n+1} + V_{n-1} C_{P_V} T_{n-1} + \lambda V_{n-1}$

energy balance

$$\cancel{H_n \frac{dm_n}{dt}} = \cancel{H_{n+1} L_{n+1}} + \cancel{H_{n-1} V_{n-1}} - \cancel{L_n H_n} - \cancel{V_n H_n}$$

$$\frac{d(H_{L_n} m_n)}{dt} = H_{L_{n+1}} \times L_{n+1} + H_{V_{n-1}} V_{n-1} - L_n H_{L_n} - V_n H_{V_n}$$

suppose, $C_p = a + bT + cT^2$

$$H = \int_{T_0}^{T} C_p \, dT = \int_{T_0}^{T} (a + bT + cT^2) \, dT$$

$$= \left[aT + \frac{bT^2}{2} + \frac{cT^3}{3} \right]_{T_0}^{T}$$

$$H = a(T - T_0) + \frac{b}{2}(T^2 - T_0^2) + \frac{c}{3}(T^3 - T_0^3)$$

$$H^V = \Sigma H_i^V y_i$$

Steps

1. from BPT (Bubble point temperatue)
   known $\rightarrow x, P$ $\rightarrow$ known from mass balance.
   Unknown $\rightarrow y^*, T$

2. $$h = \frac{y_n - y_{n-1}}{y_n^* - y_{n-1}}$$ [from here calculate actual y]

3. find $\Rightarrow H^V = \Sigma H_i^V y_i$

4. Use energy balance to find V (vapour flow rate)

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→ How to calculate H_L / H^L ...

$$\boxed{H_i^L = H_i^V - \cancel{\lambda_i}}$$

sat. sat. latent heat

$\lambda_i \Rightarrow f(T)$.

∴ Use Clausius Clapeyron eqn.

→ To calculate V assume : i. $H_n^L = 0$

ii. $H_n^L \frac{dm_n}{dt}$

iii. $H_n^L \frac{dm_n}{dt} + m_n \frac{dH_n^L}{dt}$

→ Francis-weir eqn to calculate liq flowrate

steady state

$$L_n = L_{n_0} + \frac{m_n - m_{n_0}}{\beta} \rightarrow SS$$

β = hydraulic time constant

3-6 sec

Assume $L_{n_0} = R$ (Reflux flow rate)

→ finally we can calulate V

Note: Reboiler and reflux drums are also 2 stages with 100% efficiency.