Distillation

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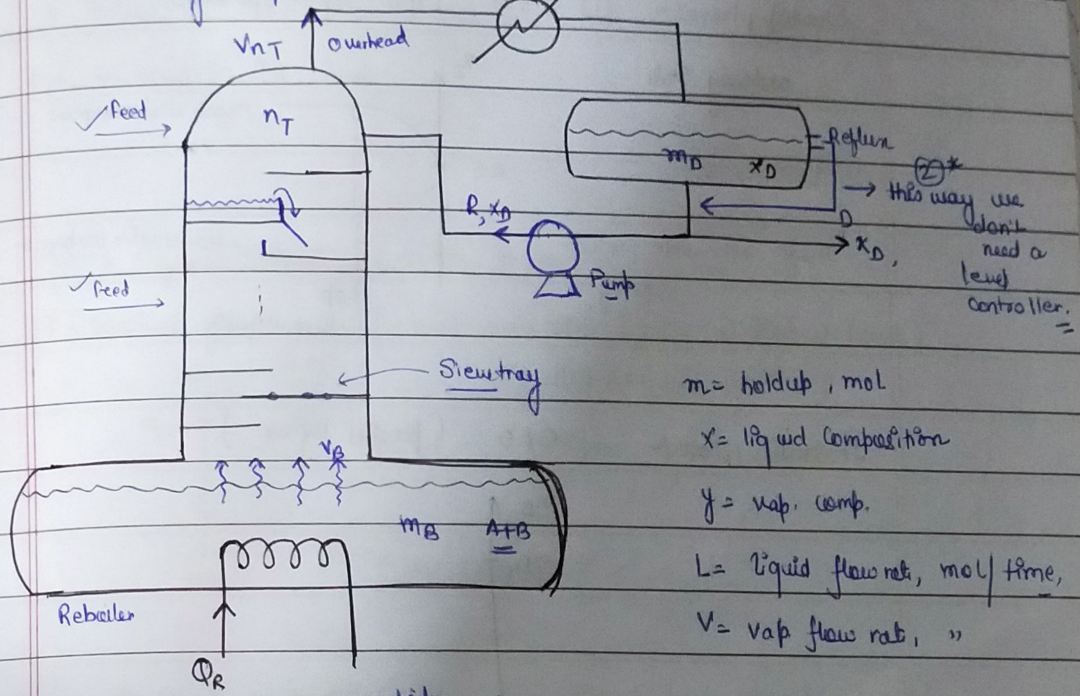
(I) Batch process :-

batch | continuous.

flexibility of batch is more vs cost.

Composition can be varied in batch.

unsteady state process.



m = holdup, mol

x = liquid composition

y = vap. comp.

L = liquid flow rate, mol/time,

V = vap flow rate, "

* fresh feed (subcooled liquid) → need some sensible heat to make it enough hot to vaporize.
(to reboiler, if)

Startup phase :-

Production phase :-

* Vapour will move up due to pressure difference.

* When the max limit pressure of column is reached, we start the condenser.

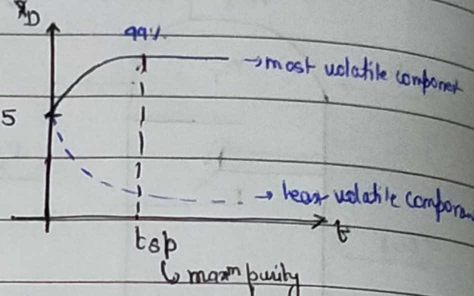
1 atm, $T_{nT} = -5°C$ – for this pressure we need refrigerant gas coolant ↓ which is costlier than water,

but 10 atm, $T_{nT} = 30°C$ – for high pr. water is used as coolant

* level controller in reflux drum can be used.
(2) *

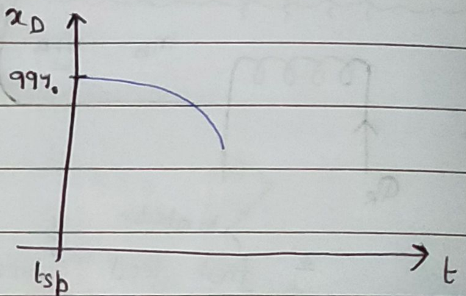
Startup phase :- (1) D = 0. (total reflux operation).

unsteady State



maxm achievable product purity

Production phase :- D ≠ 0 (partial reflux)



we will stop at whatever product composition we want, (flexible).

if → 95% → Stop at 95%

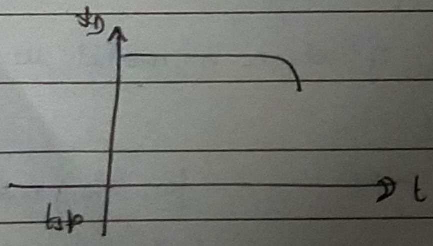
Reflux drum Size :-

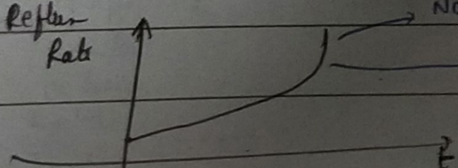
If R = 10 mol/min.

70% of Reflux drum Size should be 10-15 minutes of R mol. -

(∵ the pump may disrupt so we need to change pump).

it takes 10-15 min.





→ No lighter faction present in the column

→ * To increase R, we need a Controller.

$T_0 = A + B$

$T_1 = Ae^{\ldots} + B$

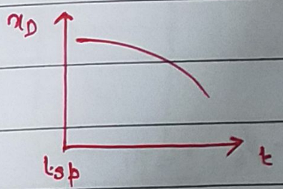
$T_0 - T_1 = A(1 - e^{\ldots})$

opt Reboiler duty is at optimum, we can't increase the duty. Since more vap. of non-volatile component would start coming too.

Amount in reboiler keeps decreasing, but content is becoming heavier so then, we need to ↑se heat.

Modes of operation for batch process:-

(I) - constant reflux ratio [- can't maintain purity at highest level].
↳ R/D ↳ purity will decrease with time.
- Open loop operation



(II) - Constant composition [- closed loop operation].

(III) Constant distillate rate. - open loop operation
- can't maintain purity.

Model developing:-

(1) Assumptions:- (i) No heat loss to surrounding. (Insulated)
(ii) Perfectly insulated process
(iii) Vapor holdup is negligible.
X (iv) heat of vaporization of component A & comp. 'B' are equal.
we will not consider this assumption.
$V_1 = V_2 = \ldots = V_n = V_B$

flaws ↳ When pressure is very high, we can't neglect vapor holdup.
↳ Q_{loss} can be added to heat equation.
(v) Liquid holdup - Variable.

Consideration: (vi) inefficient trays - (70%) [100% - ideal distillation column]

(vii) Non-ideal liquid phase.

consideration: (viii) Column Pressure (= 1 atm) + Stage $\Delta P = 0.5\,kPa$

** (ix) Perfect mixing in each tray.

(x) Volumetric holdup is constant irrespective of composition.

Equations:-

(1) Reboiler:-

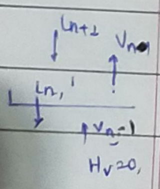
Total mole: $\frac{dm_B}{dt} = L_1 - V_B = -D$.

Energy:- $\frac{d}{dt}(m_B H_B^L) = L_1 H_1^L - V_B H_B^V + Q_R$

(2) Bottom most tray:-

$$\frac{dL_1}{dt} = L_2 + \cancel{V_B} - L_1 - \cancel{V_B} = L_2 - L_1$$

(3) n^{th} tray:-



$$\frac{dL_n}{dt} = L_{n+1} - L_n + V_{n-1} - V_n$$

$$\frac{d}{dt}(H_L x_n) = L_{n+1} x_{n+1} - L_n x_n + V_n y_n - V_{n+1} y_{n+1}$$

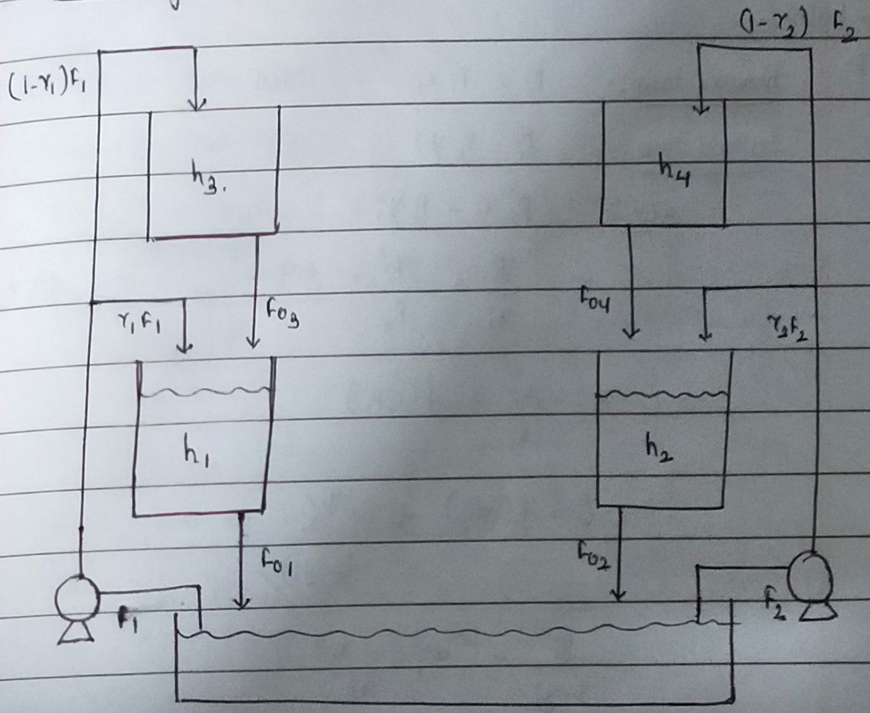
(4) top most tray:-

(5) Reflux drum

$$\frac{dm_D}{dt} = V_{nT} - R - D.$$

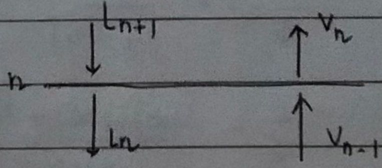
$$\frac{d}{dt}(m_D x_D) = V_{NT} y_{NT} - R x_D - D x_D.$$

4-tank System:-



Distillation:-

n^{th} plate:-



Total: $$\frac{dm_n}{dt} = L_{n+1} + V_{n-1} - L_n - V_n$$

Component: $$\frac{d(m_n x_n)}{dt} = L_{n+1} x_{n+1} + V_{n-1} y_{n-1} - L_n x_n - V_n y_n$$

Energy: $$\frac{d}{dt}(m_n H_n^L) = L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - L_n H_n^L - V_n H_n^V$$

Variables:- m, mol   x, mol fraction   T, temperature

y, mol fraction   L, mol/min   V, mol/min.

- m - can be found by total mole balance.
- z, mol fraction - can be determined by component balance.
- T : Temperature,

  ⇓

  Vapor - liquid Equilibrium [from bubble point temperature]

Bubble point:- Temp.

Raoult's law :- $p_i = P_i^\circ x_i$ --- ideal (L)

Dalton's law :- $p_i = P_t\, y_i$ --- " (V)

VLE :- $P_i^\circ x_i = P_t\, y_i$

$$K_i = \frac{y_i}{x_i} = \frac{P_i^\circ}{P_t} = \frac{\exp\left[A_i - \frac{B_i}{T+C_i}\right]}{P_t} = f(T, P_t)$$

$$\alpha_{ij} = \frac{K_i}{K_j} = f(T, P_t)$$

$$y_i = f(\alpha_{ij}) \Rightarrow \frac{y_i/x_i}{(1-y_i)/(1-x_i)} = \alpha_{ij}$$

$$\frac{y_i}{1-y_i} = \alpha_{ij}\frac{(1-x_i)}{x_i}$$

$$\frac{1-y_i}{y_i} = \frac{x_i}{\alpha_{ij}(1-x_i)}$$

$$\frac{1}{y_i} - 1 = \frac{x_i}{\alpha_{ij}(1-x_i)}$$

$$\frac{1}{y_i} = \frac{\alpha_{ij}(1-x_i) + x_i}{\alpha_{ij}(1-x_i)}$$

$$y = \frac{\alpha_{12}\, x}{1 + (\alpha_{12} - 1)\, x}$$

Case I :

Known : x_1, K_1

Unknown : y_1, y_2

$$y_1 = K_1 x_1$$

$$y_2 = 1 - y_1$$

Case 2: known : x_1 , α_{12}

unknown : y_1 , y_2

$$y_1 = \frac{\alpha_{12} x_1}{1 + (\alpha_{12} - 1) x_1}$$

$$y_2 = 1 - y_1$$

Case 3: known : x, P_t , (A_1, B_1, C_1) ✓ given

unknown : y, T

(1) T = Tassume.

(2) $P_i^o = \exp\left(A_i - \frac{B_i}{T + C_i}\right)$

(3) $y_i = \frac{x_i P_i^o}{P_t}$

(4) $|\Sigma y_i - 1| \le tol$

(5) $f(T) = \Sigma y_i - 1$, $f'(T)$

(6) $T_{new} = T_{old} - \frac{f(T)}{f'(T)}$

If liquid phase is non-ideal,

Modified Raoult's law : $P_i = P_i^o x_i \gamma_i$ --- non-ideal (liquid phase)

$P_i = P_t y_i$

$\gamma_i P_i^o x_i = P_t y_i$

| $\gamma_i = f(T, x_i)$ Binary interaction parameters are involved.
- Margule
- Var laar — UNIQUAC
- Wilson — UNIFAC
- NRTL

(1) ✓

(2) ✓

(3) $\gamma_i = f(T, x_i)$

(4) $y_i = \frac{P_i^o x_i \gamma_i}{P_t}$

(5) → (4)

(6) → (5) (7) → (6)

Non-ideal (both L + V) → Equation of State model

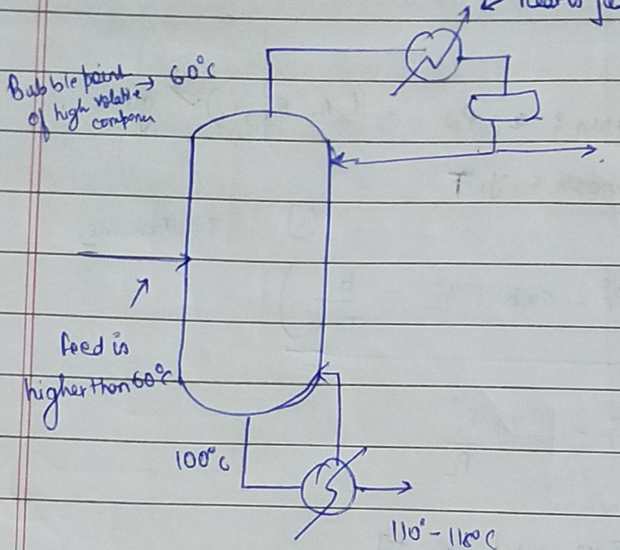
$\gamma - \phi$ -- Heterogeneous

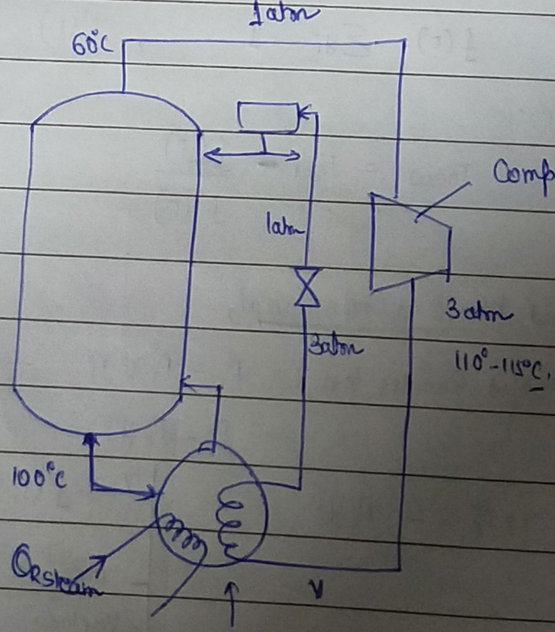
$\phi_L - \phi_V$ --- Homogenous.

Equation of State

So, $\boxed{T_L = T_V}$ — thermal eq^n

← heat is just wasted. (Economically)
↓
we can use to preheat the feed that is initially at atmospheric temp.





Cost is high.

Compression (requires high amount of elect. Energy)
↳ depends on countries.

↑ In this calculation we can consider T = dew point temp.

$\boxed{T_L = T_V}$ [thermal Eqm]

$\boxed{P_L = P_V}$ [Mechanical Eqm]

$\boxed{\mu_i^L = \mu_i^V}$ [Phase Eqm]

T, y - from bubble point temperatures.

- Liquid flow rate :- ~~L, V & 1~~

  - L: Francis-~~Wier~~ Weir Equation

$$\boxed{L_n = L_{no} + \frac{m_n - m_{no}}{\beta}}$$

Above the feed, $L_{no} = R$

below " , $L_{no} = R + F$

β, hydraulic time constant :- 3-6 sec.

- Actual 'y' :- vapor - liquid Equilibrium,

knowns: x, P_t

unknowns: y^*, T $\qquad$ y^* = found at Equilibrium.

Actual 'y' can be found by tray efficiency.

Efficiency:-

(1) Point efficiency

(2) tray efficiency

(3) Column efficiency

Murphree :- $\eta = \frac{y_n - y_{n-1}}{y^*_n - y_{n-1}}$

⇓

~~How to get y_{n-1}??~~

Column base-cum-reboiler :- 1 stage.
condenser-cum-reflux drum :- 1 stage
} 100% efficient. ∴ $y = y^*$

Reboiler - column base

$y_B = y^*$ (from bubble point calculation)

$y_1 = y_B + \eta (y_1^* - y_B)$

$\vdots$

Enthalpy:-

for a particular component → $H_i^V = \int_{T_0}^{T} C_p \, dT$: Vapor Enthalpy

$$C_p = a_1 + a_2 T + a_3 T^2 + a_4 T^3$$

$$H^V = a_1 (T - T_0) + \frac{a_2}{2}(T^2 - T_0^2) + \frac{a_3}{3}(T^3 - T_0^3) + \frac{a_4}{4}(T^4 - T_0^4)$$

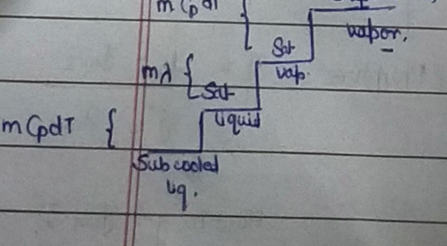
$$H_i^V = \sum_{k=1}^{4} \frac{a_k}{k}(T^k - T_0^k)$$

- $T_0 = 0$ a_k : Henley & Seader
- $T_0 = 25°C$ a_k Prausnitz → values are available component-wise

$$H_t^V = \sum H_i^V y_i$$

Actual y_i (calculated from y_i^*)

for liquids:-



Liquid Enthalpy:-

$H_i^L = H_i^V - \lambda$ → latent heat.

Clausius Clapeyron equation,

$$\frac{d(\ln P^\circ)}{dT} = \frac{\lambda}{RT^2}$$

$$\ln P^\circ = A - \frac{B}{T+C}$$

$$\lambda_i = RT^2 \left[\frac{B}{(T+C)^2}\right]$$

component wise.

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Vapor flow rate :-

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

$$m_n \frac{dH_n^L}{dt} + H_n^L \frac{dm_n}{dt} = L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - L_n H_n^L - V_n H_n^V$$

$\downarrow$ mass balance.

$$m_n \frac{dH_n^L}{dt} + H_n^L (L_{n+1} + V_{n-1} - L_n - V_n) = L_{n+1} \quad '' \quad ''$$

$$\frac{dH_n^L}{dt} = \frac{H_n^L(t+1) - H_n^L(t)}{\Delta t}$$

$\Downarrow$

So we need to use iterative method.

$$V_n(-H_n^L + H_n^V) = L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - V_{n-1} H_n^L - L_{n+1} H_n^L - m_n \frac{dH_n^L}{dt}$$

$$V_n(H_n^V - H_n^L) = L_{n+1}(H_{n+1}^L - H_n^L) \mp V_{n-1}(H_n^L - H_{n-1}^V) - m_n \frac{dH_n^L}{dt} \quad (1)$$

1. Assume V_n at $t = t$.
2. Compute x_n at $t+1$ from component balance equation.
3. Bubble point temperature, $T(t+1)$ ~~from~~
4. Compute $H(t+1) \Rightarrow \frac{dH_n^L}{dt} = \frac{H_n^L(t+1) - H_n^L(t)}{\Delta t}$
5. $V_t = V_n$
6. $V_n(t)$ from equation (1),
7. Convergence : $\left| \frac{V_n - V_t}{V_t} \right| \le tol.$

: very long Calculation

Case (1) So, Assume, $\frac{d}{dt}(m_n H_n^L) = 0$

$\Downarrow$

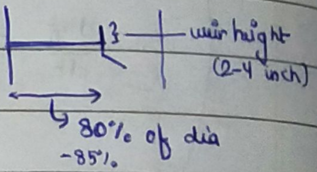
$$L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - L_n H_n^L - V_n H_n^V = 0$$

Case (II) :- $H \frac{dm_n}{dt}$ (only enthalpy constant)

Simulation Algorithm :- (for whole column)

① Input Specification :

- Feed (Composition, flow rate, quality)
- Dimension (diameter, weir dimension)



- Pressure profile.
  (Pressure drop per stage)
- η, tray efficiency.
- β, hydraulic time constant.
- C_P, coefficient.

② ODE - IVP Problem :-

- $m(0)$
- $x(0)$
- $T(0)$ (-required in Bubble point temp.)

③ Q_R and R Reflux rate.

④ Calculate BPT :- T, y^*

Actual y :- from efficiency (η)

⑤ Enthalpy calculation, :- (need T and phase composition)

vapor :- T, y

liquid :- T, x

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(6) Liquid flow rate , $L_n = L_{n0} + \frac{m_n - m_0}{\beta}$

we need reference. ($L_{n0} = R$)

(7) Vapor flow rate, V_n

(8) $m(t+1)$

$x(t+1)$

To continue Simulation, go back to step (5).

m_B, m_D - Constant } well maintained by implying level controller.

→ boiler, → condenser.

— x —

(1) $\frac{dx}{dt} = 5e^{-x^2}$, Implicit Euler (Solve)

$f = 5e^{-x^2}$

$x_{k+1} = x_k + h f_{k+1}$

$\underbrace{x_{k+1}}_{w} = \underline{x_k} + h\left[5 \exp\left(-\underbrace{x_{k+1}^2}_{w}\right)\right]$

$\underbrace{w - x_k - h(5\exp(-w^2))}_{g(w)} = 0$.

~~for~~ $g(w) = w - x_k - 5h\exp(-w^2)$ (x_k given)

⇓

Now apply another iterative method.

N-R method :- to find w at particular k. → ($w = x_{k+1}$)

$$\left[w_k^{i+1} = w_k^i - \frac{f(w_k^i)}{f'(w_k^i)} \right]$$

Boundary Value ~~Layer~~ Problem :-

Boundary Conditions :-

$$\frac{dy_k}{dx} = f_k(x, y_1, y_2, \dots, y_n)$$

$$k = 1, 2, 3, \dots$$

- Dirichlet BC :

$$y(x_m) = \beta$$

- Neumann BC :

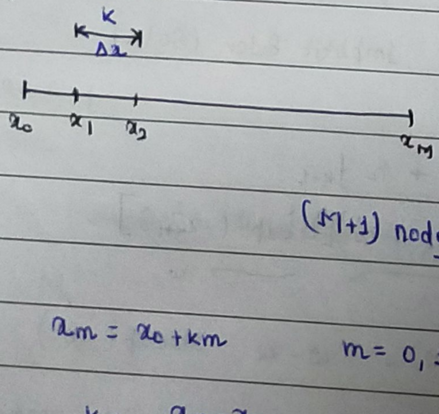
$$\left.\frac{dy}{dx}\right|_{x_m} = \beta$$

- Robin BC :

$$\beta_1 \left.\frac{dy}{dx}\right|_{x_m} + \beta_2\, y(x_m) = \beta_3$$

Methods :-

- Finite Difference method.
- Shooting method



$(M+1)$ nodes.

$$x_m = x_0 + km \qquad m = 0, 1, \dots, M$$

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

Taylor Series :-

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

$$= y_m + \left.\frac{dy}{dx}\right|_{x_m} k + O(k^2) \qquad \text{— (1)}$$

$$\left.\frac{dy}{dx}\right|_{x_m} = \frac{y_{m+1} - y_m}{k} + O(k)$$

$\boxed{x^2+0.81}$

$$y_{m-1} = y_m - \left.\frac{dy}{dx}\right|_{x_m} k + \left.\frac{d^2y}{dx^2}\right|_{x_m} \frac{k^2}{2!} + O(k^3) \quad - (\text{II})$$

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

Subtracting (I) with (II),

$$y_{m+1} - y_{m-1} = 0 + 2\left.\frac{dy}{dx}\right|_{x_m} k + O(k^3) \ldots$$

Center difference

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

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

Solution Methodology:-

1. Discretize
2. AE (Algebraic Eqn)

(I) Center Difference finite Method

Ex: 1)

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

$$x \in [a,b] \qquad y(a) = y_a \qquad y(b) = y_b$$

$x_0 \quad x_1 \quad x_m$

Discretizing:-

$$P(x)_m \left\{ \frac{y_{m+1} + y_{m-1} - 2y_m}{k^2} \right\} + q(x)_m \left\{ \frac{y_{m+1} - y_{m-1}}{2k} \right\} = r(x)_m$$

$$\left(\frac{q_m}{2k} + \frac{P_m}{k^2}\right) y_{m+1} + y_{m-1}\left(\frac{P_m}{k^2} - \frac{q_m}{2k}\right) - \left(\frac{2P_m}{k^2}\right) y_m = r_m$$

$$y_{m+1}\left(\frac{P_m}{k^2}+\frac{q_m}{2k}\right) = \left(\frac{2P_m}{k^2}\right)y_m - y_{m-1}\left(\frac{P_m}{k^2}-\frac{q_m}{2k}\right) + r_m$$

$$\cancel{y_{m+1}} = \left\{\cancel{\frac{4P_m}{P_m + kq_m}}\right\} y_m - \left\{\cancel{\frac{P_m - 2q_m}{P_m + 2q_m}}\right\} \cancel{y_{m-1}} +$$

$$y_{m+1}(2P_m + kq_m) = 4P_m y_m - y_{m-1}(2P_m - q_m k) + 2k^2 r_m$$

$m=1,$

$$y_2(2P_1 + kq_1) = 4P_1 y_1 - y_0(2P_1 - q_1 k) + 2k^2 r_1$$

$m=2,$

$$y_3(2P_2 + kq_2) = 4P_2 y_2 - y_1(2P_2 - q_2 k) + 2k^2 r_2$$

$\vdots$

$m = m-1$

$$y_m(2P_{m-1} + kq_{m-1}) = 4P_{m-1} y_{m-1} - y_{m-2}(2P_{m-1} - q_{m-1}k) + 2k^2 r_{m-1}$$

Total m-1 eq^n will be formed,

$$\begin{bmatrix} -4P_1 & (2P_1+kq_1) & 0 & \cdots & 0 \\ (2P_2-kq_2) & -4P_2 & (2P_2+kq_2) & \cdots & 0 \\ \vdots & & & & \\ \vdots & & & & \\ 0 & \cdots & 0 & (2P_{m-1}-kq_{m-1}) & -4P_{m-1} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{m-1} \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$

Here, we have considered, Dirichlet B.C's,

$E_0 \quad E_1 \quad E_2 \quad E_3 \quad E_4$

(a) Dirichlet e.g.:-

E.g.:-

$$-\frac{d^2u}{dx^2} = 2 \qquad x \in [0,1]$$

$u_0 = 0 \qquad\qquad u_6 = 0$

$u(0) = 0 \qquad\qquad u(1) = 0. \qquad\qquad m = 6.$

$x_0 \quad x_1 \quad x_2 \quad x_3 \quad x_4 \quad x_5 \quad x_6$

$$k = \frac{x_m - x_0}{m} = \frac{1-0}{6} = 1/6$$

$$-\frac{(u_{m+1} + u_{m-1} - 2u_m)}{k^2} = 2$$

$$u_{m+1} + u_{m-1} - 2u_m = -2k^2$$

$m = 1,$

$$u_2 + \cancel{u_0}^{0} - 2u_1 = -2k^2$$

$m = 2,$

$$u_3 + u_1 - 2u_2 = -2k^2$$

$m = 3,$

$$u_4 + u_2 - 2u_3 = -2k^2$$

$m = 4,$

$$u_5 + u_3 - 2u_4 = -2k^2$$

$m = 5,$

$$\cancel{u_6}^{0} + u_4 - 2u_5 = -2k^2$$

$\therefore u_1 = 0.138889$

$u_2 = 0.22222$

$u_3 = \cancel{0.19444}\ 0.250001$

$u_4 = 0.222226$

$u_5 = 0.138891$

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}_{5\times5} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}_{5\times1} = -2k^2 \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\left\{ -\frac{d^2u}{dx^2} = 2 \Rightarrow \frac{du}{dx} = -2x + a \Rightarrow u = -x^2 + ax + b \right.$$

$x = 0 \quad u = 0 \Rightarrow b = 0$

$x = 1 \quad u = 0 \Rightarrow a = 1.$

$u = -x^2 + x$

x	U_a (Analytical)	U_n (numerical)
0	0	0
1/6	0.138888	0.138889
2/6	0.222222	0.22222
3/6	0.25	0.250006
4/6	0.22222	0.222226
5/6	0.13888	0.138891
6/6	0	0

(b) Neumann B.C. :-

E.g.:- $$\frac{d^2T}{dx^2} = \frac{hP}{KA}(T - T_0)$$ [fin Problem]

$m = 4$ $\frac{hP}{KA} = 1$

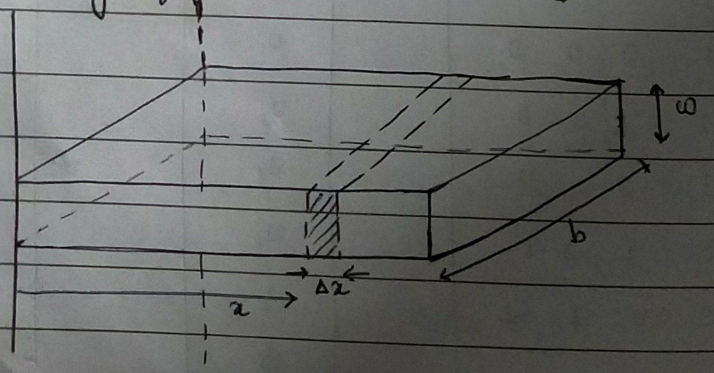
h: convective heat transfer coefficient.

P: Perimeter.

A: conductive heat transfer Area.

T_0: Ambient Temperature.

l: length of fin. T_ω: wall temp.



B.C. :- $T(x=0) = T_\omega$ $x = l = 4$.

$$\left.\frac{\partial T}{\partial x}\right|_{x=l} = 0$$

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Non-dimensionalizing,

Let, $\theta = \frac{T - T_0}{T_\omega - T_0}$ $\quad \xi = \frac{x}{l}$ and $H = \sqrt{\frac{hPl^2}{KA}}$

$$\frac{d^2T}{dx^2} = (T_\omega - T_0)\frac{d^2\theta}{dx^2} = \frac{(T_\omega - T_0)}{l^2}\frac{d^2\theta}{d\xi^2}$$

$$\frac{d\theta}{dx} = \frac{dT}{dx} \times \frac{1}{(T_\omega - T_0)}$$

$$(T - T_0) = \theta(T_\omega - T_0)$$

$$\frac{(T_\omega - T_0)}{l^2}\frac{d^2\theta}{d\xi^2} = \frac{hP}{KA}\theta(T_\omega - T_0)$$

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

$\xi = 0$, $x = 0$ $\quad T = T_\omega$, $\theta = 1$

$$\left.\frac{dT}{dx}\right|_{x=l} = \left.\frac{d\theta}{dx}\right|_{x=l}(T_\omega - T_0) \Rightarrow \left.\frac{d\theta}{dx}\right|_{x=l} = 0$$

$$\Rightarrow \left.\frac{d\theta}{d\xi}\right|_{\xi=1} = 0$$

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

$\xi = 0, \theta = 1$

$\xi = 1, \left.\frac{d\theta}{d\xi}\right| = 0$

$$K = \frac{\xi_m - \xi_0}{m} = \frac{1-0}{4} = \frac{1}{4}$$

Applying Center Finite difference,

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

$H^2 = \frac{hP}{kA} l^2$ $\quad l = 4 \quad \frac{hP}{kA} = 1$

$H^2 = 16 \quad k^2 = 1/16$

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

$$\theta_{m+1} = 3\theta_m - \theta_{m-1}$$

$m = 1,$

$$\theta_2 = 3\theta_1 - \theta_0 \qquad \Big| \; \theta_0 = 1$$

$m = 2,$

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

$m = 3,$

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

$m = 4,$

$$\theta_5 = 3\theta_4 - \theta_3$$

- considering θ_5 so to take its value from Another B.C.

from another B.C.,

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=1} = 0$$

At $m = 4,$

$$\frac{\theta_{m+1} - \theta_{m-1}}{2k} = 0$$

$$\theta_5 - \theta_3 = 0 \Rightarrow \theta_5 = \theta_3.$$

$\therefore$

$$2\theta_3 = 3\theta_4$$

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

$$\theta_2 = 3\theta_1 - 1$$

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

$$+\frac{7\theta_3}{3} = +\theta_2 \quad \Rightarrow \quad \theta_3 = \frac{3\theta_2}{7}$$

$$\frac{18\theta_2}{7} = \theta_1 \quad \Rightarrow \quad \theta_2 = \frac{7\theta_1}{18}$$

$$\frac{7\theta_1}{18} - 3 = -1$$

$$\frac{47}{18}\theta_1 = 1 \quad \Rightarrow \quad \theta_1 = \frac{18}{47} = 0.38297$$

$$\theta_2 = 0.148936$$

$$\theta_3 = 0.063829$$

$$\theta_4 = 0.042553$$

Analytical Sol^n :-

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

$$(m^2 - 16)\theta = 0$$

$$\theta = c_1 e^{-4\xi} + c_2 e^{4\xi}$$

BCs

$$\xi = 0 \qquad \theta_0 = 1.$$

$$c_1 + c_2 = 1$$

$$\frac{d\theta}{d\xi} = -4c_1 e^{-4\xi} + 4c_2 e^{4\xi}$$

At $\xi = 1$, $\frac{d\theta}{d\xi} = 0$

$$0 = -4c_1 e^{-4} + 4c_2 e^{4}$$

$$c_1 e^{-4} = c_2 e^{4}$$

$$c_1 = c_2 e^{8} \quad \Rightarrow \quad c_2 = \frac{1}{1+e^8} \quad c_1 =$$

$$c_2 = 3.35 \times 10^{-4} \quad c_1 =$$

$$\theta = 0.999\, e^{-4\xi} + 3.35 \times 10^{-4}\, e^{4\xi}$$

At, $\xi = 0$, $\theta_0 = 0.999335$

$\xi = 1/4$ $\theta_1 = 0.36842$

$\xi = 2/4$ $\theta_2 = 0.13767$

$\xi = 3/4$ $\theta_3 = 0.05646$

$\xi = 1$ $\theta_4 = 0.036587$

ξ	θ_n	θ_a	Error
0	1	0.999335	6.65×10^{-4}
$1/4$	0.38297	0.3684	1.4×10^{-2}
$2/4$	0.148936	0.13767	1.1×10^{-2}
$3/4$	0.063829 ~~0.05646~~	0.05646	7.4×10^{-3}
$4/4 = 1$	0.042553	0.036587	6×10^{-3}

'm' value Should be taken in large steps.

(C) Robin – neumann B.C.
tubular

Ex: An isothermal ~~batch~~ reactor : Robin BC + Non-linear Case:-

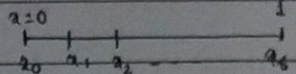
$$\frac{1}{Pe}\frac{d^2c}{dx^2} - \frac{dc}{dx} - D_a c^2 = 0$$

Pe = Peclet no. = 6

Da = Damkohler no. = $2 = \frac{kV}{F}$

$x \in [0, 1]$

$$\left.\frac{dc}{dx}\right|_{x=0} = Pe\,(c-1) \quad \text{--- Robin BC}$$



$$\left.\frac{dc}{dx}\right|_{x=1} = 0 \quad \text{--- Neumann BC}$$

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

$M = 6$

$$\frac{1}{6}\left[\frac{C_{m+1} + C_{m-1} - 2C_m}{K^2}\right] - \left[\frac{C_{m+1} - C_{m-1}}{2K}\right] - 2C_m^2 = 0$$

$$6\left[C_{m+1} + C_{m-1} - 2C_m\right] - 3\left[C_{m+1} - C_{m-1}\right] - 2C_m^2 = 0$$

$$3C_{m+1} + 9C_{m-1} - 12C_m = 2C_m^2$$

$m = 0$,

$$3C_1 + 9C_{-1} - 12C_0 = 2C_0^2 \quad \text{— (I)}$$

$m = 1$,

$$3C_2 + 9C_0 - 12C_1 = 2C_1^2 \quad \text{— (II)}$$

$m = 2$,

$$3C_3 + 9C_1 - 12C_2 = 2C_2^2 \quad \text{— (III)}$$

$m = 3$,

$$3C_4 + 9C_2 - 12C_3 = 2C_3^2 \quad \text{— (IV)}$$

$m = 4$,

$$3C_5 + 9C_3 - 12C_4 = 2C_4^2 \quad \text{— (V)}$$

$m = 5$,

$$3C_6 + 9C_4 - 12C_5 = 2C_5^2 \quad \text{— (VI)}$$

$m = 6$,

$$3C_7 + 9C_5 - 12C_6 = 2C_6^2 \quad \text{— (VII)}$$

B.C.s:- (I) $\left.\frac{dc}{dx}\right|_{x=0} = 6(c-1)$

$\frac{\cancel{c_0} - \cancel{c_1}}{2\times\cancel{1/6}} \neq 6\,\cancel{(c_1-1)}$

$m=0,$

$\frac{c_1 - c_{-1}}{2\times 1/6} = 6(c_0-1)$

$c_1 - c_{-1} = 2(c_0-1).$

$c_{-1} = c_1 - 2(c_0-1)$

Now from eq (I),

$3c_1 + 9(c_1 - 2(c_0-1)) - 12c_0 = 2c_0^2$

$12c_1 - 30c_0 + 18 = 2c_0^2$

Eq^n (I) reduces to:- $-30c_0 + 12c_1 = 2c_0^2 - 18$

B.C.:- (II) $\left.\frac{dc}{dx}\right|_{x=1} = 0$

$m=6,$ $\frac{c_7 + c_5 - 2c_6}{k^2} = 0$

$c_7 = 2c_6 - c_5$

Eq^n (IV) reduces to:-

$3(2c_6 - c_5) + 9c_5 - 12c_6 = 2c_6^2$

$6c_5 - 6c_6 = 2c_6^2$

H.W. — Solve by Simultaneous N-R

from Octave Code

taking $c_0 = c_1 = c_2 = c_3 = c_4 = c_5 = c_6 = 0.$

After 5 iterations.

Ans. $c_0 = 0.83009$ $c_1 = 0.69007$ $c_2 = 0.58748$ $c_3 = 0.50978$

$c_4 = 0.44993$ $c_5 = 0.40535$ $c_6 = 0.38114.$

(d) Robin - Robin :-

$$P(x)\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x) \qquad x \in [a,b]$$

$$a_0\, y(a) + b_0\, y'(a) = c_0 \quad \text{--- Robin} \qquad \cancel{y_0' = y'(a) =}$$

$$a_1\, y(b) + b_1\, y'(b) = c_1 \quad \text{--- Robin}$$

1st B.C. :-

$$y(x+K) = y(x) + K y'(x) + \frac{K^2}{2!} y''(x) + \frac{K^3}{3!} y'''(x) + \cdots$$

$$y(x+2K) = y(x) + 2K y'(x) + \frac{(2K)^2}{2!} y''(x) + \frac{(2K)^3}{3!} y'''(x) + \cdots$$

$$y(x+2K) - 4y(x+K) = -3y(x) - 2Ky'(x) + O(K^3)$$

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

$m=0$, $$y_0' = y'(a) = \frac{-3y_0 + 4y_1 - y_2}{2K}$$

a ——— b

$x_0 \quad x_1 \quad x_2 \quad \ldots \quad x_m$

↳ Put in B.C.I.

Steps :-

(1) Use center difference on main equation from $m=1$ to $m-1$.

(2) $m=0$ for 1st B.C.

(3) $m=M$ for 2nd B.C.

for $m=0$, $$\left(a_0 - \frac{3b_0}{2K}\right)y_0 + \frac{2b_0}{K}y_1 - \frac{b_0}{2K}y_2 = c_0$$

B.C. II :-

$$y(x-K) = y(x) - Ky'(x) + \frac{K^2}{2!}y''(x) \mp \frac{K^3}{3!}y'''(x) + \cdots$$

$$y(x-2K) = y(x) - 2Ky'(x) + \frac{(2K)^2}{2!}y''(x) - \frac{(2K)^3}{3!}y'''(x) + \cdots$$

$$y(x-2K) - 4y(x-K) = -3y(x) + 2Ky'(x) + O(K^3)$$

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

$m = M$,

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

Put it in B.C. (2),

$$\frac{b_1}{2k} y_{M-2} - \frac{2b_1}{k} y_{M-1} + \left(a_1 + \frac{3b_1}{2k}\right) y_M = c_1$$

Main Eqn :-

$m = 1, 2, \ldots, M-1$: $(2P_m - kq_m)y_{m-1} - 4P_m y_m + (2P_m + kq_m)y_{m+1} = 2k^2 r_m$

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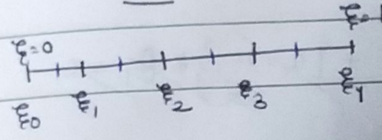
① Cooling fin System :- (Previous Neumann B.C. Example)

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

$$\theta(0) = 1$$

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=1} = 0$$

$M = 4$



ξ	Analytical	Numerical
0	1	1
0.25	0.3687	0.3830
0.50	0.1378	0.1489
0.75	0.0565	0.0638
1.0	0.0366	0.0425

Error was so large.

no. of nodes = 5

So, we can either increase M or, Mesh Refinement (nodes ↑)

Method (I) * Mesh Refinement

No. of new nodes = 2×No. of old nodes − 1

$M = 8$. $\qquad$ $M = 4$

$$\theta = 0.999\, e^{-4\xi} + 3.35\times10^{-4}\, e^{4\xi}$$

for $M = 8$,

ξ	Analytical	Numerical (Given)
0	0.999335	1
0.125	0.60647	0.6100
0.25	0.36842	0.3725
0.375	0.2244	0.2281
0.5	0.13767	0.1407
0.625	0.08608	0.0885
0.75	0.056466	0.0584
0.875	0.04126	0.0429
1.0	0.03658	0.0381

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Method (II) : Numerical Solution:- (with no fictious node).

$$\theta_{m-1} + \theta_{m+1} - 3\theta_m = 0 \qquad m = 1, 2, 3$$

BC-2 (formula derived from ~~robin-robin B.C.~~), $m = 4$,

$K = \frac{1-0}{4} = \frac{1}{4}$

$m = 4$,

$$\cancel{\frac{b_1}{2K}\theta_2 - \frac{2b_1}{K}\theta_3 + \left(a_1 + \frac{3b_1}{2K}\right)\theta_4 = c_1}$$

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=1} = 0$$

$a_1 = 0$ $\quad \cancel{b_1 = 1}$ $\quad \cancel{c_1 = 0}$

$\cancel{2\theta_2 - 8\theta_3}$

$m = 4$,

using Robin-Robin derivation for B.C. II,

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

$$\theta'_m = \frac{\theta_{m-2} - 4\theta_{m-1} + 3\theta_m}{2K}$$

At $\xi = 1$, (m=4) $\quad \theta'_4 = 0$

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

$$\theta_0 + \theta_2 - 3\theta_1 = 0$$

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

$$\theta_2 + \theta_4 - 3\theta_3 = 0 \longrightarrow \theta_3 - 2\theta_4 = 0 \Rightarrow \theta_3 = 2\theta_4$$

$\theta_2 = 5\theta_4$

$\theta_4 = \frac{\theta_2}{5}$

Solving,

$\theta_0 = 1$ $\qquad \theta_2 - 3\theta_1 = -1$

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

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

$$\theta_2 = \frac{5}{2}\theta_3 \quad \Rightarrow \quad \theta_3 = \frac{2\theta_2}{5}$$

$$\frac{1+\theta_2}{3} + \frac{2\theta_2}{5} - 3\theta_2 = 0.$$

$$\frac{1}{3} + \theta_2\left(\frac{1}{3} + \frac{2}{5} - 3\right) = 0.$$

$$\frac{1}{3} + \theta_2\left(\frac{5+6-45}{15}\right) = 0.$$

$$\theta_2 = \frac{-5}{11-45} = \frac{5}{34} = 0.1470$$

$$\theta_3 = 0.0588$$

$$\theta_4 = 0.0294$$

$$\theta_1 = 0.38233$$

ξ	Numerical	
0	1	
1/4	0.38233	
2/4	0.1470	
3/4	0.0588	
4/4	0.029412	not much improvement.

$\therefore$ Mesh refinement is better option.

① Gravity Pendulum:-

$$\frac{d^2\theta}{dt^2} + \beta \sin\theta = 0 \qquad \beta = 10$$

$t=0 \quad t_1 \quad t_2 \quad \cdots \quad t=1$

$m=0$ t_0 $\qquad$ $m=M$ t_M

$\theta_0 \qquad \theta(t=0) = 0.7$

$\theta_M \qquad \theta(t=1) = 0.5 \qquad M$

use central difference method,

$$\frac{\theta_{m+1} + \theta_{m-1} - 2\theta_m}{K^2} + \beta \sin\theta_m = f(\theta_m)$$

N-R method (for multivariable):-

$$x_{m+1} = x_m - J_m^{-1} f_m$$

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \vdots & & & \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix}$$

Back to prb:-

$$\theta_{m+1} + \theta_{m-1} - 2\theta_m + \beta K^2 \sin\theta_m = K^2 f(\theta_m) = K^2 f_m$$

$m=1 \Rightarrow \quad \theta_0 - 2\theta_1 + \theta_2 + K^2 \beta \sin\theta_1 = K^2 f_1$

$$\frac{\partial f_1}{\partial \theta_1} = \frac{-2 + K^2 \beta \cos\theta_1}{K^2}$$

$$\frac{\partial f_1}{\partial \theta_2} = \frac{1}{K^2}$$

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$m=2 \Rightarrow \theta_3 + \theta_1 - 2\theta_2 + \beta K^2 \sin\theta_2 = K^2 f_2$

$\frac{\partial f_2}{\partial \theta_1} = +1/K^2$

$\frac{\partial f_2}{\partial \theta_2} = \frac{-2 + \beta K^2 \cos\theta_2}{K^2}$

$\frac{\partial f_3}{\partial \theta_3} = 1/K^2$

$\beta = 0.7$

$M = 6$

$\theta_6 = 0.5$

$\theta_0 = 0.7$

$K = \frac{2\pi}{6} = \pi/3$

$\underline{M=6}$

$m=3 \Rightarrow \theta_4 + \theta_2 - 2\theta_3 + \beta K^2 \sin\theta_3 = K^2 f_3$

$m=4 \Rightarrow \theta_5 + \theta_3 - 2\theta_4 + \beta K^2 \sin\theta_4 = K^2 f_4$

$m=5 \Rightarrow \theta_6 + \theta_4 - 2\theta_5 + \beta K^2 \sin\theta_5 = K^2 f_5$

$\cancel{\frac{\partial f_3}{\partial \theta_1} = \frac{-2}{K^2}}$ $\quad \frac{\partial f_3}{\partial \theta_2} = +\frac{1}{K^2}$ $\quad \frac{\partial f_3}{\partial \theta_3} = \frac{-2 + \beta K^2 \cos\theta_3}{K^2}$

$\frac{\partial f_4}{\partial \theta_4} = 1/K^2$

$\frac{\partial f_4}{\partial \theta_3} = +1/K^2$ $\quad \frac{\partial f_4}{\partial \theta_4} = \frac{-2 + \beta K^2 \cos\theta_4}{K^2}$ $\quad \frac{\partial f_4}{\partial \theta_5} = 1/K^2$

$\frac{\partial f_5}{\partial \theta_4} = +\frac{1}{K^2}$ $\quad \frac{\partial f_5}{\partial \theta_5} = \frac{-2 + \beta K^2 \cos\theta_5}{K^2}$

After Solving

$\theta_1 = 1.3455$ $\quad \theta_2 = 1.7203$ $\quad \theta_3 = 1.8204$

$\theta_4 = 1.6513$ $\quad \theta_5 = 1.2054$.

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Shooting Method :-

- 2^{nd} or higher order BVP. — B.C.'s given

1. BVP → IVP.
   ↳ But we need I.C.'s
2. IVP Solver.
3. Convergence check. → Linear Interpolation / → Secant | N-R method,

~~Eg:-~~

General :- B.V.P.

$$\frac{d^2y}{dx^2} = F\left(x, y, \frac{dy}{dx}\right)$$

B.C.'s : $y(x=a) = \alpha$

$y(x=b) = \beta$

$x=a$ $x=b$

Steps :-

1. $y = y_1$

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

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

$y_1(x=a) = \alpha = y_{10}$

$y_2(x=a) = y_{20}$ (Not known, So Assume the value)

$x=a$ $x=b$ — and check the final value if matching or not

y_{1m} $y_{1(m+1)}$ — calculate by Explicit Euler | difference b/w the actual value and Explicit Euler value is converg...

y_{2m} $y_{2(m+1)}$

(2) Explicit Euler

$$y_{1,m+1} = y_{1m} + k y_{2m}$$

$$y_{2,m+1} = y_{2m} + k f_m$$

(3) $| y_{1,m+1} - y_1(x \pm b) | \leq tol$??

{Shooting + Explicit Euler + Linear Interpolation}

E.g:

$$\frac{d^2 y}{dx^2} = 5y + 10x(1-x) \Rightarrow f_m = 5 y_{1m} + 10 x_m (1 - x_m)$$

B.C.'s : $y(0) = 0$ $\quad M = 3 \quad K = \frac{9-0}{3} = 3$

$y(9) = 0 \quad tol = 10^{-3}$

$$y_2 = \frac{dy_1}{dx} \qquad y = y_1$$

y=0 ... y=0

x=0, x=3, x=6, x=9

$y_1^0 \quad y_1^1 \quad y_1^2 \quad y_1^3$

$$\frac{dy_2}{dx} = 5y_1 + 10x(1-x)$$

$y_{10} = 0$ $\qquad$ Initial guess for $y_{20} = 4$.

$y_{20} = 4.$

$$y_1^{m+1} = y_1^m + K y_2^m$$

$$y_2^{m+1} = y_2^m + K f_m$$

$$y_1^1 = y_1^0 + K y_2^0 = 0 + 3 \times 4 = 12$$

$$y_2^1 = y_2^0 + K f_0 = 4 + 3 \times (5 \times 0 + 10 \times 0 (1 - 0)).$$

$$= 4 \cancel{+ 3t}$$

$$y_1^2 = y_1^1 + K y_2^1 = 12 + 3 \times 4 = 24$$

$$y_2^2 = 4 + 3 \times (5 \times 12 + 10 \times 3 (1-3))$$

$$= 4 + 3 \times (60 - 60) = 4$$

$y_1^3 = y_1^2 + K y_2^2 \quad = 24 + 3\times 4 = 36$

$y_2^3 = \cancel{y_2^2}^{\,4} + 3\times (5\times 24 + 10\times 6\times(1-6))$

$= -536$

- high difference $|y_1^3 - y_1(9)|$

Step 3:-

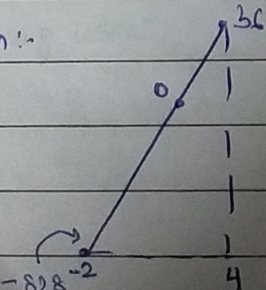
$|y_1(9) - y(9)| = 36 > tol.$

Let, $y_{20} = -2$

y_1	y_2
0	-2
-6	-2
-12	-272
-828	-

∴ Our value lie in b/w somewhere -2 & 4. (for initial guess of y_2^0)

Linear interpolation :-



$$\frac{-828-36}{-2-4} = \frac{y-36}{x-4}$$

$y=0$

$x = ?$

$$x = -\frac{36}{144} + 4$$

$x = 3.75$

∴ Initial guess should be,

$y_2^0 = 3.75$.

	y_1	y_2
1.	0	3.75
2.	11.25	3.75
3.	22.5	-7.5
4.	0	-570

$$y_1^4 - y(9) = 0$$

If ~~we~~ conv. part need to solve by Secant method,

$$y_0(x=a) = \alpha$$

$$y_0(x=b) = \beta$$

$$\cancel{y_2^0(x=0)=0}$$

$y_2^0(x=0) = s^0$ – ~~assumed~~ where, $s^0 = \dfrac{\beta-\alpha}{b-a}$

Guess Value :- s^0, s^1 (we need two guess values for Secant method)

s^1 : Another Guess value we need to assume, arbitrarily.

Secant :-

$$s^{i+1} = s^i - \frac{s^i - s^{i-1}}{f^i - f^{i-1}} \times f^i$$

(s^1 above s^i, s^0 above s^{i-1})

for Convergence,

$$y_1(b,s) - \beta = f.$$

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Shooting Method :- (Re-Cap)

BVP : $$\frac{d^2y}{dx^2} = f\left(x, y, \frac{dy}{dx}\right)$$

B.C's : $$y(x=0) = \alpha$$
$$y(x=1) = \beta$$

1st Step :- Transform to IVP. $y = y_1$

$$\frac{dy_1}{dx} = y_2 \quad -\text{(I)}$$

$$\frac{dy_2}{dx} = f(x, y_1, y_2) \quad -\text{(II)}$$

I.C's : $y_1(x=0) = \alpha$ --- B.C.1.

$y_2(x=0) = s$ --- assumed

2nd Step :- IVP Solver.

3rd Step :- convergence check

$$|y_1(1,s) - \beta| < tol$$

$$g = y_1(1,s) - \beta$$

- Generate new Guess,

(I) Secant : $$s^{i+1} = s^i - \frac{s^i - s^{i-1}}{g(s^i) - g(s^{i-1})} g(s^i) \quad \text{--- secant.}$$

$$= s^i - \frac{s^i - s^{i-1}}{y_1(1,s^i) - y_1(1,s^{i-1})} [y_1(1,s^i) - \beta]$$

$$s^0 = \frac{\beta - \alpha}{1-0} = \beta - \alpha$$

$$s^1 = y_2(0) \quad \text{[Assume value].}$$

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(II) N-R method :-

$$s^{i+1} = s^i - \frac{g(s^i)}{g'(s^i)}$$

$$= s^i - \frac{g(s^i)}{\frac{d}{ds}(y_1(1,s^i))\Big|_{s=s^i}}$$

But here,

$$\frac{dy_1}{ds} = ??$$

Let $\frac{\partial y_1}{\partial s} = y_3(x,s)$

$\frac{\partial y_2}{\partial s} = y_4(x,s)$

we can write,

- $\frac{dy_3}{dx} = \frac{d}{dx}\left(\frac{\partial y_1}{\partial s}\right) = \frac{\partial}{\partial s}\left(\frac{dy_1}{dx}\right)$

$$\frac{dy_3}{dx} = \frac{\partial y_2}{\partial s} = y_4 \quad \text{— (iii)}$$

- $\frac{dy_4}{dx} = \frac{d}{dx}\left(\frac{\partial y_2}{\partial s}\right) = \frac{\partial}{\partial s}\left(\frac{dy_2}{dx}\right) = \frac{\partial f}{ds}$

$$\frac{\partial f(x, y_1, y_2)}{\partial s}$$

$(x \neq f(s))$

$$\therefore \frac{dy_4}{dx} = \frac{\partial}{\partial s} f(x, y_1, y_2) = \frac{\partial f}{\partial x} \times \cancel{\frac{\partial x}{\partial s}}^{0} + \frac{\partial f}{\partial y_1} \times \frac{\partial y_1}{\partial s} + \frac{\partial f}{\partial y_2} \times \frac{\partial y_2}{\partial s}$$

$$\frac{dy_4}{dx} = \frac{\partial f}{\partial y_1} \cdot y_3 + \frac{\partial f}{\partial y_2} \cdot y_4 \quad \text{— (iv)}$$

$\therefore$ we have 4 equations in total,

$$\frac{dy_1}{dx} = y_2 \quad \text{— (i)} \qquad \frac{dy_3}{dx} = y_4 \quad \text{— (iii)}$$

$$\frac{dy_2}{dx} = f(x, y_1, y_2) \quad \text{— (ii)} \qquad \frac{dy_4}{dx} = y_3 \frac{\partial f}{\partial y_1} + y_4 \frac{\partial f}{\partial y_2} \quad \text{— (iv)}$$

$\therefore$ 4 variable 4 eqn,

So we need 4 guess values,

$y_1(0) = \alpha \qquad y_2(0) = s \qquad y_3(0) = 0 \qquad y_4(0) = 1$

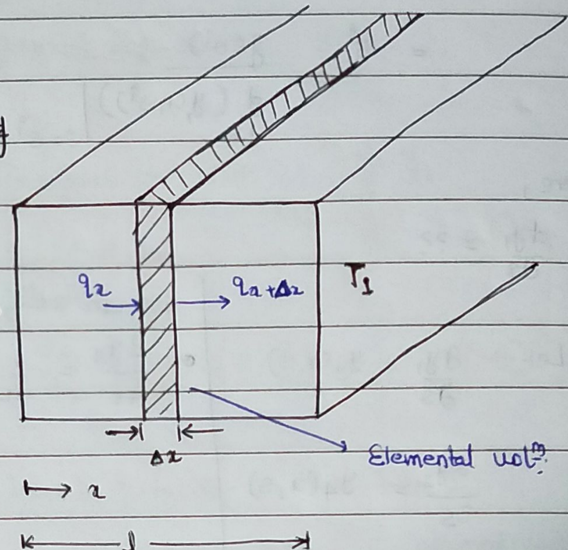
$y_1(0,s) = \alpha \Rightarrow \frac{\partial y_1}{\partial s} = 0 = y_3(0)$ || $y_2(0,s) = s \Rightarrow \frac{\partial y_2}{\partial s} = 1 = y_4(0)$

$$\therefore \frac{\partial y_1}{\partial s}(1, s^{(i)}) = y_3(1, (s^{(i)}))$$

Example :-

Case Study

heat generation = $\dot{q}$
(per unit vol^m)



Steady State, 1-D heat conduction.

Input + heat Generation = Output

$$q_x + \dot{q}(A\Delta x) = q_{x+\Delta x}$$

Let, $\dot{q} = 0$ (-No heat Generation).

$$\therefore q_x = q_{x+\Delta x}$$

$$-KA\left.\frac{dT}{dx}\right|_x + KA\left.\frac{dT}{dx}\right|_{x+\Delta x} = 0$$

$\lim_{\Delta x \to 0}$. $\Rightarrow$ $$\frac{d}{dx}\left(K\frac{dT}{dx}\right) = 0$$

to make it non-linear,

$$K = f^n(T)$$

$$K = K_0 + K_1(T - T_0)$$

Non-Dimensionalizing, $\theta = \frac{T - T_0}{T_1 - T_0}$ $\quad \xi = \frac{x}{l}$ $\quad a = \frac{K_1}{K_0}(T_1 - T_0)$

$a = 1$ (Given)

$$\frac{dK}{dx} \times \frac{dT}{dx} + K\frac{d^2T}{dx^2} = 0.$$

$$K = K_0 + K_1 (T - T_0)$$

$$\frac{dK}{dx} = K_1 \frac{dT}{dx}$$

$$\therefore \quad K_1 \left(\frac{dT}{dx}\right)^2 + K\frac{d^2T}{dx^2} = 0.$$

$$K\frac{d^2T}{dx^2} = -K_1 \left(\frac{dT}{dx}\right)^2$$

$$\frac{d^2T}{dx^2} = \frac{-K_1}{K}\left(\frac{dT}{dx}\right)^2$$

$$\frac{d\theta}{dx} = \frac{1}{T_1 - T_0}\frac{dT}{dx} \Rightarrow \frac{d^2T}{dx^2} = (T_1 - T_0)\frac{d^2\theta}{dx^2}$$

$$\frac{(T_1 - T_0)}{l^2}\frac{d^2\theta}{d\xi^2} = \frac{-K_1}{K_0 + K_1(T - T_0)}\left(\frac{dT}{dx}\right)^2$$

$$\left(\frac{T_1 - T_0}{l^2}\right)\frac{d^2\theta}{d\xi^2} = \frac{-K_1/K_0}{1 + \frac{K_1}{K_0}(T - T_0)} \times \frac{(T_1 - T_0)^2}{l^2}\left(\frac{d\theta}{d\xi}\right)^2$$

B.V.P :-

$$\frac{d^2\theta}{d\xi^2} = \frac{-a}{1 + a\theta}\left(\frac{d\theta}{d\xi}\right)^2$$

B.C.'s :-

$x = 0$	$T = T_0$	$\Rightarrow$	$\xi = 0$	$\theta = 0$	$\theta(\xi = 0) = 0$
$x = l$	$T = T_1$	$\Rightarrow$	$\xi = 1$	$\theta = 1$	$\theta(\xi = 1) = 1$

#1 Now, Solving with Shooting + Explicit + Secant.

$$\theta = \theta_1$$

$$\frac{d\theta_1}{d\xi} = \theta_2 \qquad \frac{d\theta_2}{d\xi} = \frac{-a}{1 + a\theta_1}\theta_2^2 = \frac{-a\theta_2^2}{1 + a\theta_1}$$

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$M = 10.$

$$\frac{d\theta_1}{d\xi} = \theta_2 \qquad \frac{d\theta_2}{d\xi} = \frac{-a\theta_2^2}{1+a\theta_1} = \frac{-\theta_2^2}{1+\theta_1}$$

$\theta_1(\xi=0) = 0$

$\theta_2(\xi=0) = s$

$s^0 \quad s^1$

$K = \frac{1-0}{10} = 0.1$

$s^0 = \frac{1-0}{1-0} = 1 \qquad s^1 = 1.2$ (Assume).

S/7

Step 2:-

$$\theta_1^{i+1} = \theta_1^i + \left(\frac{d\theta_1}{d\xi}\right)^i \times K$$

$$\theta_2^{i+1} = \theta_2^i + \left(\frac{d\theta_2}{d\xi}\right)^i \times K$$

Step 3:-

$$s^2 = s^1 - \frac{s^1 - s^0}{g(s^1) - g(s^0)} g(s^1)$$

$g = \theta_1(1, s) - 1$

last ξ

(for next s^3, we need to do step '2' again so as to get last ξ value).

2. Shooting + Explicit Euler + N-R

$M = 10 \;;\; a = 1$

$$\frac{d\theta_1}{d\xi} = \theta_2 \quad -(1)$$

$$\frac{d\theta_2}{d\xi} = \frac{-\theta_2^2}{1+\theta_1} \quad -(11)$$

$y^{i+1} = y^{i} + Ky'$

$$\frac{d\theta_3}{d\xi} = \theta_4 \quad \text{— (iii)}$$

$$\cancel{\frac{d\theta_4}{d\xi} = \theta_4 \frac{\partial f}{d\xi} + \theta_4}$$

$$\frac{d\theta_4}{d\xi} = \theta_3 \frac{\partial f}{\partial \theta_1} + \theta_4 \frac{\partial f}{\partial \theta_2}$$

$$\begin{cases} \theta_1(0) = 0 \\ \theta_2(0) = S \\ \theta_3(0) = 0 \\ \theta_4(0) = 1 \end{cases}$$

$\Downarrow$

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Coupled - BVP

$$\frac{d^2y}{dx^2} = f_1(y_1, y_2) \quad -(1)$$

$$\frac{d^2y_2}{dx^2} = f_2(y_1, y_2) \quad -(2)$$

$x_0 \quad x_1 \quad x_2 \quad - - - - - - \quad x_M$

$y_{10} \quad y_{11} \quad - - - - - - \quad y_{1m}$

$y_{20} \quad y_{21} \quad - - - - - - \quad y_{2m}$

B.C.'s : On y_1 and y_2

$$z = \begin{bmatrix} y_{10} \\ y_{11} \\ \vdots \\ y_{1m} \\ \hline y_{20} \\ y_{21} \\ \vdots \\ y_{2m} \end{bmatrix} = \begin{bmatrix} z_0 \\ z_1 \\ \vdots \\ z_M \\ \hline z_{m+1} \\ \vdots \\ z_{2M+1} \end{bmatrix}$$

$$z_m = \begin{cases} y_{1m} & m \in [0, M] \\ y_{2m-(m+1)} & m \in [M+1, 2M] \end{cases}$$

Discretizing Equation (1),

$$\frac{y_{1,m+1} - 2y_{1,m} + y_{1,m-1}}{k^2} = f_1(y_{1,m}, y_{2,m})$$

$$\frac{z_{m+1} - 2z_m + z_{m-1}}{k^2} = f_1(z_m, z_{m+M+1})$$

$$z_{m-1} - 2z_m + z_{m+1} - k^2 f_1(z_m, z_{m+M+1}) = g(z_m)$$

$$z_{m+1} = z_m - \frac{g(z_m)}{g'(z_m)} \quad --- \text{N-R}$$

From Eqn (ii),

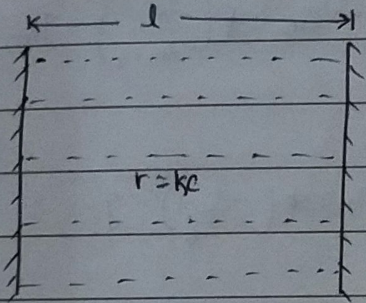
$$\frac{y_{2,m+1} - 2y_{2,m} + y_{2,m-1}}{k^2} = f_2(y_{1m}, y_{2m})$$

$$\frac{Z_{m+M+2} - 2Z_{m+M+1} + Z_{m+M}}{K^2} = f_2(Z_m, Z_{m+M+1})$$

$$Z_{m+M} - 2Z_{m+M+1} + Z_{m+1+M+1} - K^2 f_2(Z_m, Z_{m+M+1}) = g_{m+M+1}$$

E.g.:-

Reaction - diffusion System



Dimensionless,

$\bar{c} = c/c_0$, $\bar{T} = T/T_0$

$\bar{x} = x/l$ $\alpha = E/RT_0$

$c(x=0) = 0$ $c(x=l) = C_0$ $\varphi = \sqrt{\frac{k_0 l^2}{D}}$ $\gamma = \frac{k_0 C_0 (\Delta H_r) l^2}{K T_0}$

$T(x=0) = T_0$ $T(x=l) = T_0$

Assumption :- Steady state, 1-D, Only Conduction, 1st Order rxn,

- Model :-

$$D\frac{d^2c}{dx^2} - k_0 \exp\left(-\frac{E}{RT}\right)c = 0 \quad -(1)$$

$$K\frac{d^2T}{dx^2} + (-\Delta H_r) k_0 \exp\left(-E/RT\right) c = 0 \quad -(2)$$

- Model eqn in dimensionless form:-

$$\frac{d^2\bar{c}}{d\bar{x}} = \varphi^2 \bar{c} \exp\left(-\frac{\alpha}{\bar{T}}\right) \quad --(3)$$

$\bar{c}(\bar{x}=0) = 0$

$\bar{c}(\bar{x}=1) = 1$

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$$\frac{d^2\bar{T}}{d\bar{x}^2} = \gamma\,\bar{c}\,\exp\left(-\frac{\alpha}{\bar{T}}\right) \; ; \quad \bar{T}(\bar{x}=0) = \bar{T}(\bar{x}=1) = 1 \qquad (4)$$

$\underline{M=4}$

$\bar{x}=0$ $\qquad\qquad\qquad\qquad$ $\bar{x}=1$

$$0 = \begin{matrix} \bar{c}_0 & \bar{c}_1 & \bar{c}_2 & \bar{c}_3 & \bar{c}_4 \\ z_0 & z_1 & z_2 & z_3 & z_4 \end{matrix} = 1$$

$$1 = \begin{matrix} \bar{T}_0 & \bar{T}_1 & \bar{T}_2 & \bar{T}_3 & \bar{T}_4 \\ z_5 & z_6 & z_7 & z_8 & z_9 \end{matrix} = 1$$

For eqn (3),

$$\frac{\bar{c}_{m+1} + \bar{c}_{m-1} - 2\bar{c}_m}{k^2} = \varphi^2\,\bar{c}_m\,\exp\left(-\frac{\alpha}{\bar{T}_{m+5}}\right)$$

$$z_{m+1} + z_{m-1} - 2z_m - k^2\varphi^2 z_m \exp\left(\frac{-\alpha}{z_{m+5}}\right) = g_m$$

- $m=1$

$$z_2 + \cancel{z_0}^{\,0} - 2z_1 - k^2\varphi^2 z_1 \exp\left(\frac{-\alpha}{z_6}\right) = g_1$$

$$\frac{\partial g_1}{\partial z_1} = -2 - k^2\varphi^2 \exp\left(-\frac{\alpha}{z_6}\right) = g_{11}$$

$$\frac{\partial g_1}{\partial z_2} = 1 = g_{12}$$

$$\frac{\partial g_1}{\partial z_6} = -k^2\varphi^2 z_1 \exp\left(-\frac{\alpha}{z_6}\right) \times \frac{\alpha}{z_6^2} = g_{16}$$

- $m=2$

$$z_3 + z_1 - 2z_2 - k^2\varphi^2 z_2 \exp\left(-\frac{\alpha}{z_7}\right) = g_2$$

$$\frac{\partial g_2}{\partial z_1} = 1 = g_{21} \qquad \frac{\partial g_2}{\partial z_2} = -2 - k^2\varphi^2 \exp\left(-\frac{\alpha}{z_7}\right) = g_{2}$$

$$\frac{\partial g_2}{\partial z_3} = 1 = g_{23} \qquad \frac{\partial g_2}{\partial z_7} = -k^2\varphi^2 z_2 \frac{\alpha}{z_7^2} \exp\left(\right.$$

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• $m = 3$,

$$\cancel{z_4} + z_2 - 2z_3 - K^2 \varphi^2 z_3 \exp\left(\frac{-\alpha}{z_8}\right) = g_3$$

$$\frac{\partial g_3}{\partial z_2} = 1 = g_{32} \qquad \frac{\partial g_3}{\partial z_3} = -2 - K^2\varphi^2 \exp\left(-\frac{\alpha}{z_8}\right) = g_{33}$$

$$\cancel{\frac{\partial g_3}{\partial z_4} = 1 = g_{34}} \qquad \frac{\partial g_3}{\partial z_8} = -K^2\varphi^2 z_3 \frac{\alpha}{z_8^2} \exp\left(-\frac{\alpha}{z_8}\right) = g_{38}$$

For eq^n (4),

$$\frac{d^2 \bar{T}}{d\bar{q}^2} = \gamma \bar{c} \exp\left(-\frac{\alpha}{\bar{T}}\right)$$

m starts from 5

$$\frac{\bar{T}_{m+1} + \bar{T}_{m-1} - 2\bar{T}_m}{K^2} = \gamma \bar{c}_m \exp\left(-\frac{\alpha}{\bar{T}_m}\right)$$

$m \to m + M + 1$ (for $\bar{T}$)

$$\frac{z_{m+6} + z_{m-4} - 2z_{m+5}}{K^2} = \gamma z_m \exp\left(\frac{-\alpha}{z_{m+5}}\right)$$

$$g_{m+5} = z_{m+6} + z_{m+4} - 2z_{m+5} - \gamma z_m K^2 \exp\left(-\frac{\alpha}{z_{m+5}}\right)$$

• $m = 1$,

$$g_6 = z_7 + \underbrace{z_5}_{=1} - 2z_6 - \gamma z_1 K^2 \exp\left(-\frac{\alpha}{z_6}\right)$$

$$\frac{\partial g_6}{\partial z_1} = -\gamma K^2 \exp\left(-\frac{\alpha}{z_6}\right) = g_{61} \qquad \frac{\partial g_6}{\partial z_6} = -2 - \gamma z_1 K^2 \frac{\alpha}{z_6^2} \exp\left(-\frac{\alpha}{z_6}\right) = g_{66}$$

$$\frac{\partial g_6}{\partial z_7} = 1 = g_{67}$$

• $m = 2$,

$$g_7 = z_8 + z_6 - 2z_7 - \gamma z_2 K^2 \exp\left(-\frac{\alpha}{z_7}\right)$$

$$\frac{\partial g_7}{\partial z_8} = 1 = g_{78} \qquad \frac{\partial g_7}{\partial z_6} = 1 = g_{76} \qquad \frac{\partial g_7}{\partial z_2} = -\gamma K^2 \exp\left(-\frac{\alpha}{z_7}\right) = g_{72}$$

$$\frac{\partial g_7}{\partial z_7} = -2 - \gamma z_2 K^2 \frac{\alpha}{z_7^2} \exp\left(-\alpha/z_7\right) = g_{77}$$

$m=3,$

$$g_8 = z_9 + z_7 - 2z_8 - r z_3 k^2 \exp\left(\frac{-\alpha}{z_8}\right)$$

$\therefore$

$$\begin{bmatrix} z_{1,n+1} \\ z_{2,n+1} \\ z_{3,n+1} \\ z_{6,n+1} \\ z_{7,n+1} \\ z_{8,n+1} \end{bmatrix} = \begin{bmatrix} z_{1,n} \\ z_{2,n} \\ z_{3,n} \\ z_{6,n} \\ z_{7,n} \\ z_{8,n} \end{bmatrix} - \underbrace{\begin{bmatrix} g_{11} & g_{12} & 0 & g_{16} & 0 & 0 \\ g_{21} & g_{22} & g_{23} & 0 & g_{27} & 0 \\ 0 & g_{32} & g_{33} & 0 & 0 & g_{38} \\ g_{61} & 0 & 0 & g_{66} & g_{67} & 0 \\ 0 & g_{72} & 0 & g_{76} & g_{77} & g_{78} \\ 0 & 0 & g_{83} & 0 & g_{87} & g_{88} \end{bmatrix}^{-1}}_{J} \times \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_6 \\ g_7 \\ g_8 \end{bmatrix}$$

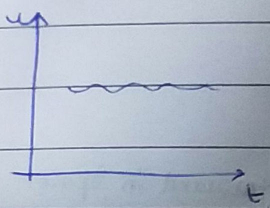
Assume the values (initial for, $n=0$)

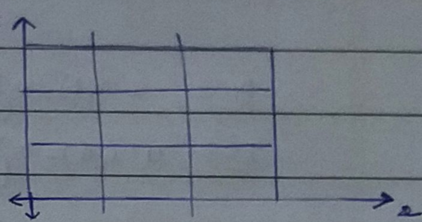
Partial Differential Equations:

ODE	PDE
① one independent variable	① more than one independent variable.
② Either IC's or ~~BVP's~~ BC's	② Here we need both IC & BC. (IBVP) Problem.

$\dot{u} = f(t, u)$

$u(t=0) = u_0$





Finite Difference :- (Methods).

→ Leap-frog

→ Method of Lines

→ Lax-Friedrichs

→ Crank-Nicolson

Steps : ① M (Along Space) N (for time.)

$\Delta x = K$ $\Delta t = h$

② Replace the equations with their finite difference approx.

③ Algebraic equations.

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Ex-1: One way wave equation:

$$u_t + a u_x = f(t)$$

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad \text{(Let)}$$

Space: $x_m = x_0 + km \qquad m = 0, 1, \dots, M$

time: $t_n = t_0 + hn \qquad n = 0, 1, \dots, N$

BC: $u(0, t) = g(t)$

IC: $u(x, 0) = g(x)$

(I) Apply: Forward in time and forward in space. (FTFS)

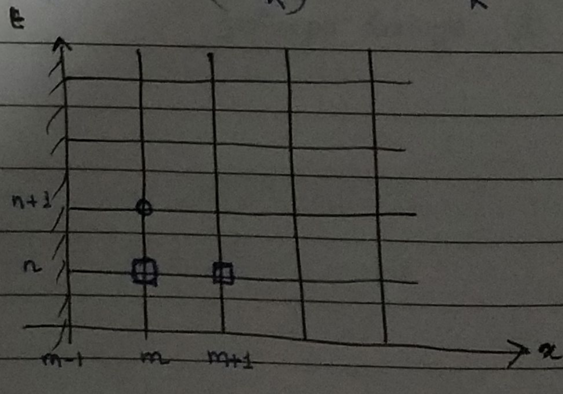
$$\frac{\partial u}{\partial t} = \frac{u(x_m, t_{n+1}) - u(x_m, t_n)}{h} = \frac{u_{m,n+1} - u_{m,n}}{h}$$

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

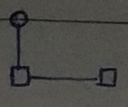
$$\frac{u_{m,n+1} - u_{m,n}}{h} = -a\frac{(u_{m+1,n} - u_{m,n})}{k} + O(k,h)$$

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

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



Computational molecule :-



○ → to find
□ → need information

(II) BTBS,

$$\frac{\partial u}{\partial t} = \frac{u(x_m, t_n) - u(x_m, t_{n-1})}{h} = \frac{u_{m,n} - u_{m,n-1}}{h}$$

$$\frac{\partial u}{\partial x} = \frac{u(x_m, t_n) - u(x_{m-1}, t_n)}{k} = \frac{u_{m,n} - u_{m-1,n}}{k}$$

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

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

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

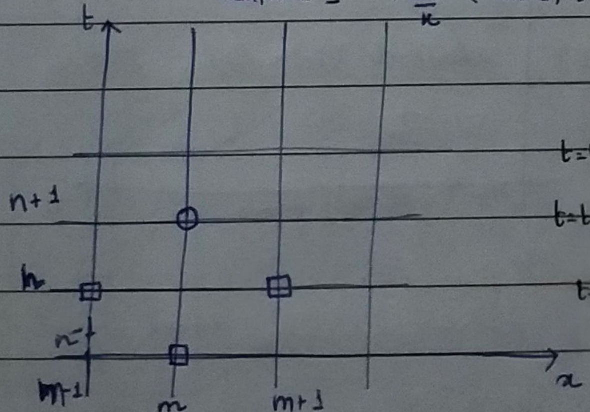
(III) CTCS,

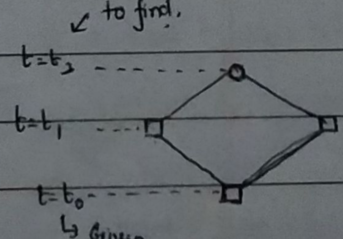
$$\frac{\partial u}{\partial t} = \frac{u_{m,n+1} - u_{m,n-1}}{2h} \qquad \frac{\partial u}{\partial x} = \frac{u_{m+1,n} - u_{m-1,n}}{2k}$$

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

$$u_{m,n+1} + \frac{ah}{k}u_{m+1,n} = u_{m,n-1} + \frac{ah}{k}u_{m-1,n}$$

$$u_{m,n+1} = +\frac{ah}{k}(u_{m-1,n} - u_{m+1,n}) + u_{m,n-1}$$





so, we need to find 't_1'
we can have it from FTFS,

Ex-2: Non-linear IBVP:-

$$\frac{\partial u}{\partial t} = \left(\frac{\partial u}{\partial x}\right)^2 + u\frac{\partial^2 u}{\partial x^2}$$

B.C.'s : $u(0,t) = t$

$u(1,t) = 1+t$

I.C. : $u(x,0) = x$ $\qquad 0 \le x \le 1$

$M = 10$ $\qquad h = 0.0001$, $\qquad k = \frac{1-0}{10} = 0.1$

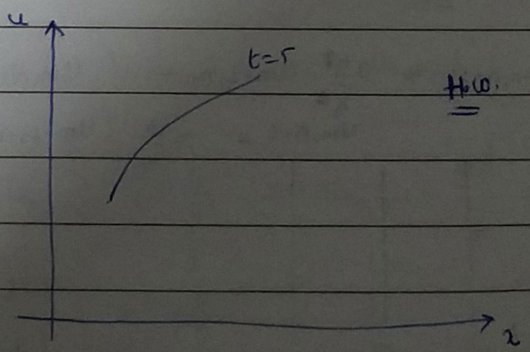
find at $\rightarrow$ $t = 0, 5, 10$.

CTCS to main Eqn :

$$\frac{u_{m,n+1} - u_{m,n-1}}{2h} = \left(\frac{u_{m+1,n} - u_{m-1,n}}{2k}\right)^2 + u_{m,n}\left(\frac{u_{m+1,n} + u_{m-1,n} \ldots}{k^2}\right.$$

FTFS to main Eqn,

$$\frac{u_{m,n+1} - u_{m,n}}{h} = \left(\frac{u_{m+1,n} - u_{m,n}}{k}\right)^2 + u_{m,n}\Big($$



How plot??

(II) Method of Lines :-

- FTFS @ 1st - order Accurate
- BTBS @ 1st - order Accurate
- CTCS @ 2nd order Accurate.

Computational Steps :

① Discretize ~~to~~ the spatial domain.

$x_0 \quad x_1 \quad - - - - - - - \quad x_M$

② Convert PDE → a set of ODE's

③ Integrate the ODEs @ BCs
IC

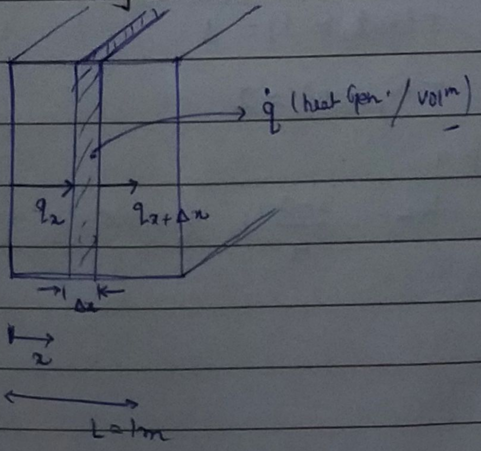
Ex :- One way wave eqn :

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

$$\frac{dU_m}{dt} = -a\,\frac{U_{m+1} - \cancel{2U_m +} U_{m-1}}{2h} \quad \text{[central finite difference]}$$

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

Examples: unsteady ~~State~~ heat Conduction (1-D)



q = heat transfer rate.

$\dot{q}$ = rate of heat generation / vol

l = total length

A = heat transfer Area.

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$$q_x - q_{x+\Delta x} + \dot{q}(V) = \rho C_p V \frac{dT}{dt}$$

$$\frac{q_x - q_{x+\Delta x}}{V} + \dot{q} = \rho C_p \frac{dT}{dt}$$

$$\lim_{\Delta \to 0} \frac{q_x - q_{x+\Delta x}}{A \, \Delta x} + \dot{q} = \rho C_p \frac{dT}{dt}$$

$$-\frac{1}{A}\frac{dq}{dx} + \dot{q} = \rho C_p \frac{dT}{dt}$$

$$K \frac{d^2T}{dx^2} + \dot{q} = \rho C_p \frac{dT}{dt}$$

let, $\dot{q} = 0.$

$$\frac{\partial^2 T}{\partial x^2} = \frac{\rho C_p}{K} \frac{\partial T}{\partial t}$$

$$\frac{\partial T}{\partial t} = \frac{K}{\rho C_p} \frac{\partial^2 T}{\partial x^2}$$

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

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

$M = 4.$

B.C's: $T(x=0, t=t) = 0$

$T(x=1, t=t) = 1$ $\quad L = 1\,m$

$T(x, t=0) = 2$

$M = 4.$

$k = \frac{1-0}{4} = \frac{1}{4} = 0.25$ $\quad \alpha = 0.00188$

~~T (t = 25)~~

$h = 0.025$ (Given)

$$f(T_{m,n}) = \alpha \left\{ \frac{T_{m+1,n} + T_{m-1,n} - 2T_{m,n}}{K^2} \right\}$$

$$T_{m,n+1} = T_{m,n} + h f(T_{m,n}).$$

$n =$

$T(t = 25) = ??$

'Forward in Time and Central in Space'.

$m = 1,$

$$T_{1,n+1} = T_{1,n} + h f(T_{1,n})$$

$$f(T_{1,n}) = \alpha \left\{ \frac{T_{2,n} + T_{0,n} - 2T_{1,n}}{K^2} \right\}$$

Now, vary $n = 0, 1, 2, \ldots, N-1$.

$m = 2,$

⋮

H.W. ??

Ex: 3 Reaction - diffusion System

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + R(c, x)$$

- Pure diffusion process : $R = 0$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$ [Fick's Second Law].

- $R = c(1-c)$: Fisher's equation.
- $R = c(1-c)(c-\alpha)$: Combustion theory.
  $0 < \alpha < 1$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + c(1-c)(c-\alpha)$$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + c(1-c)(c-\alpha)$$

$$\frac{dc_m}{dt} = D\left(\frac{c_{m+1} + c_{m-1} - 2c_m}{K^2}\right) + c_m(1-c_m)(c_m-\alpha)$$

$D = 1$

$\alpha = 0.5$

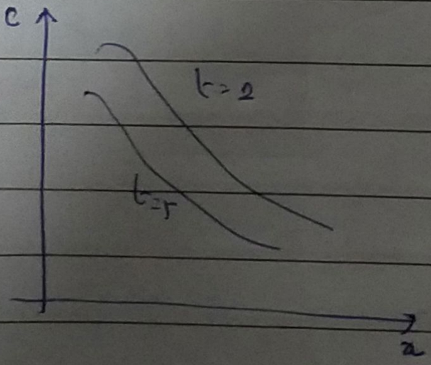
$K = 1 \quad (M = 10)$

$h = 0.005$

B.C.'s : $\begin{cases} c(0, t) = 1 \\ c(10, t) = 0 \end{cases}$ $\quad 0 \le x \le 10$

I.C.'s : $c(x, 0) = \begin{cases} 0 & x < 5 \\ 1 & x \ge 5 \end{cases}$

H.W.



Plot for
↓
t = 5, 8, 10.

Lax - Friedrichs

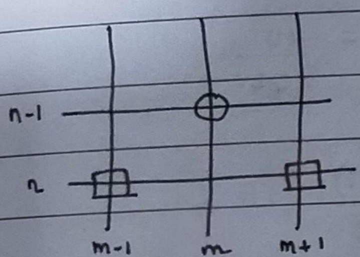
$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

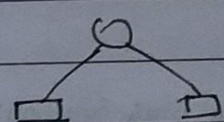
FTCS: $$\frac{u_{m,n+1} - u_{m,n}}{h} = -a\,\frac{u_{m+1,n} - u_{m-1,n}}{2K}$$

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

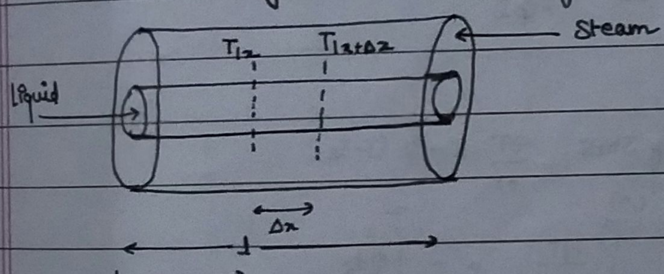
$$u_{m,n+1} = \frac{1}{2}\left(u_{m+1,n} + u_{m-1,n}\right) - \frac{ah}{2K}\left(u_{m+1,n} - u_{m-1,n}\right)$$

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





Ex: unsteady state heat Exchanger



Assumptions:-
- No heat loss
- properties are constant (ρ, C_p)
- Steam (T_s) constant
- No radial variation of Temperature
- Process fluid flows at constant v
- No heat accumulation in the walls

$$\rho v C_p \frac{\pi D^2}{4} T|_x - \rho v C_p \frac{\pi D^2}{4} T|_{x+\Delta x} + U\pi D\Delta x\left(T_{st} - T|_x\right) = \frac{d}{dt}\left(\rho \pi \frac{D^2}{4}\Delta x\, C_p\, T|_x\right)$$

$$-\rho v C_p \frac{\pi D^2}{4}\frac{dT}{dx} + U\pi D\left(T_{st} - T\right) = \frac{d}{dt}\left(\rho \pi \frac{D^2}{4} C_p T\right)$$

$$-\frac{\rho v C_p D}{4}\frac{dT}{dx} + Q = \frac{\rho D C_p}{4}\frac{dT}{dt}$$

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial x} + \frac{4Q}{\rho C_p D}$$

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial x} + \frac{4U(T_{st}-T)}{\rho C_p D}$$

$$\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x} = \frac{4U(T_{st}-T)}{\rho C_p D}$$

$$A\Delta x \rho C_p \left[T|_{t+\Delta t} - T|_t\right] = A v \rho \Delta t C_p T|_x + Q\Delta t(\pi D \Delta x) - A v \rho \Delta t C_p T|_{x+\Delta x}$$

$$\phi = \frac{4U}{\rho C_p D v}$$

Steady State Equation:

$$v\frac{\partial T}{\partial x} = \frac{4U(T_{st}-T)}{\rho C_p D}$$

IBVP: $\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x} = \frac{4U}{\rho C_p D}(T_{st}-T)$

IC: $T(x,0)$

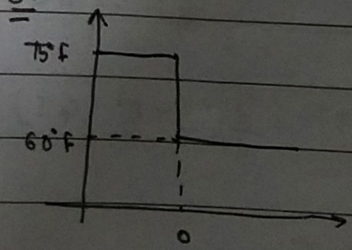
Steady State $\frac{\partial T}{\partial x} = -\phi(T-T_{st})$

$$\int_{T(0,0)}^{T(x,0)} \frac{dT}{T-T_{st}} = -\int_0^x \phi\, dx$$

$$\ln\left(\frac{T(x,0)-T_{st}}{T(0,0)-T_{st}}\right) = -\phi x$$

$$T(x,0) = T_{st} + (T(0,0)-T_{st})\, e^{-\phi x}$$

BC



$T(0,t) = 60°F$ $\qquad T(0,0) = 75°F$

$L = 12ft$ $\qquad k = L/M = 0.3$

$M = 40$ $\qquad h = \frac{k}{v} = 0.1$

$V = \cancel{3ft}/2$ ft/s $\quad T_r = 250°F$

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Process Stream Water $\quad C_p = 1\ \mathrm{Btu}/\mathrm{lb}^\circ\mathrm{F} \quad D = 0.5\,\mathrm{ft} \quad \rho = 62.4 \quad U = 0.2$

$$\frac{T_{m,n+1} - T_{m,n}}{h} = -v\,\frac{T_{m+1,n} - T_{m-1,n}}{k} + \frac{4U}{\rho C_p D}(T_{st} - T_{m,n})$$

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

$$T_{m,n+1} = -\frac{hv}{k}(T_{m+1,n} - T_{m-1,n}] + \frac{4Uh}{\rho C_p D}(T_{st} - T_{m,n}) + T_{m,n}$$

$$T_{m,n+1} = -\frac{hv}{k}(T_{m+1,n} - T_{m-1,n}] + \frac{1}{2}(T_{m+1,n} + T_{m-1,n}) + \frac{4Uh}{\rho C_p D}\left[T_{st} - \frac{1}{2}(T_{m+1,n} + T_{m-1,n})\right]$$

$$= \frac{4UhT_{st}}{\rho C_p D} + \frac{T_{m+1,n}}{2}\left[1 - \frac{4Uh}{\rho C_p D} - \frac{hv}{k}\right] + \frac{T_{m-1,n}}{2}\left[1 - \frac{4Uh}{\rho C_p D} + \frac{hv}{k}\right]$$

$$= \frac{25}{39} + \frac{T_{m+1,n}}{2}\left[1 - \frac{1}{390} - 1\right] + \frac{T_{m-1,n}}{2}\left[1 + 1 - \frac{1}{390}\right]$$

$$= \frac{T_{st}}{390} - \frac{T_{m+1,n}}{780} + T_{m-1,n}\times\frac{779}{780}$$

$$= aT_{st} + bT_{m+1,n} + cT_{m-1,n}$$

$a = 0.0025641$

$b = -0.00128205$

$c = 0.998718$

$t = 0, 1, 5$ sec

$T = ?$

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Lax - Friedrichs :-

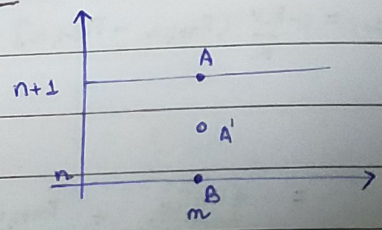
Ex :- $$\frac{\partial u}{\partial t} = \left(\frac{\partial u}{\partial x}\right)^2 + u\frac{\partial^2 u}{\partial x^2}$$

$$\frac{u_{m,n+1} - u_{m,n}}{h} = \left(\frac{u_{m+1,n} - u_{m-1,n}}{2k}\right)^2 + u_{m,n}\left(\frac{u_{m+1,n} + u_{m-1,n}}{k^2}\right.$$

Second spatial derivative will get cancelled.

Crank - Nicolson Method :-

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



(wave) $$\left(\frac{\partial u}{\partial t}\right)_{m,n+\frac{1}{2}} = -a\left(\frac{\partial u}{\partial x}\right)_{m,n+\frac{1}{2}}$$

$$\left(\frac{\partial u}{\partial t}\right)_{m,n+\frac{1}{2}} = \frac{u_{m,n+1} - u_{m,n}}{h} + O(h^2)$$

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

$$\left(\frac{\partial u}{\partial x}\right)_{m,n+\frac{1}{2}} = \frac{1}{2}\left[\frac{u_{m+1,n+1} - u_{m-1,n+1}}{2k} + \frac{u_{m+1,n} - u_{m-1,n}}{2k}\right]$$

Remarks:

1) 2^{nd} order accurate

2) Implicit method, unconditionally stable.

$\frac{u_{m,n+1} - u_{m,n+1}}{h} + \frac{u_{m,n} - (u_{m,n-1})}{h}$

Eg:- unsteady state heat conduction, u

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \qquad u \to \text{temp.}$$

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

B.C.: $u(0,t) = 0 \qquad u(l,t) = 1$

$u_{0,1} \mid u_{0,2} \mid u_{0,3} \cdots \mid u_{0,5}$

I.C.: $u(x,0) = 2$

$u_{0,0}, \; u_{1,0} \quad u_{2,0} \quad u_{3,0} \quad u_{4,0} \quad u_{5,0} \quad u_{6,0}.$

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

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

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

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

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

$M = 6$, ~~(both ...)~~

$m = 1, 2, \ldots, 5$

(I) $r\, u_{0,n+1} - (2+2r)\, u_{1,n+1} + r\, u_{2,n+1} = -r\, u_{2,n} + (2r-2)\, u_{1,n} - r\, u_{0,n}$

(II) $r\, u_{1,n+1} - (2+2r)\, u_{2,n+1} + r\, u_{3,n+1} = -r\, u_{3,n} + (2r-2)\, u_{2,n} - r\, u_{1,n}$

(III) $r\, u_{2,n+1} - (2+2r)\, u_{3,n+1} + r\, u_{4,n+1} = -r\, u_{4,n} + (2r-2)\, u_{3,n} - r\, u_{2,n}$

(IV) $r\, u_{3,n+1} - (2+2r)\, u_{4,n+1} + r\, u_{5,n+1} = -r\, u_{5,n} + (2r-2)\, u_{4,n} - r\, u_{3,n}$

(V) $r\, u_{4,n+1} - (2+2r)\, u_{5,n+1} + r\, u_{6,n+1} = -r\, u_{6,n} + (2r-2)\, u_{5,n} - r\, u_{4,n}$

$u_{0,n+1} = 0 \qquad u_{6,n+1} = 2 \qquad$ ~~$n = 0 \to 4$~~ $\quad n \to 1, \ldots, 4$

$$\begin{bmatrix} -(2+2r) & r & 0 & 0 & 0 \\ r & -(2+2r) & r & 0 & 0 \\ 0 & r & -(2+2r) & r & 0 \\ 0 & 0 & r & -(2+2r) & 0 \\ 0 & 0 & 0 & r & -(2+2r) \end{bmatrix} \begin{bmatrix} u_{1,n+1} \\ u_{2,n+1} \\ u_{3,n+1} \\ u_{4,n+1} \\ u_{5,n+1} \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \\ \\ \end{bmatrix}$$

Elliptic PDE

General : $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = H(x,y)$ --- Poisson

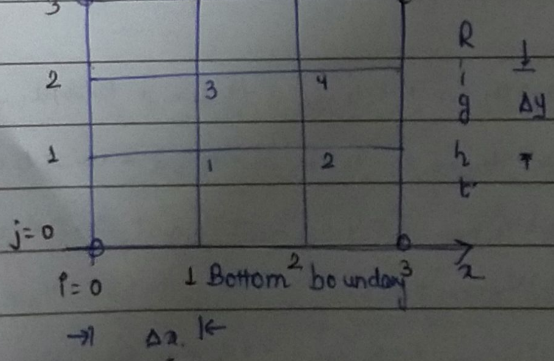
$H(x,y)$ — Source.

B.C.s : $u(x,0) = u_1$ --- Bottom

$u(0,y) = u_2$ -- left

$u(x,1) = u_3$ --- Top

$u(1,y) = u_4$ --- Right.



Computational Steps :-

(1) Discretize the domain

$\Delta x = x_{i+1} - x_i$ $\boxed{\Delta x = \Delta y = K}$

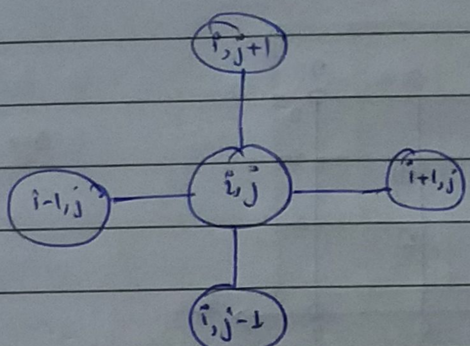
$\Delta y = y_{j+1} - y_j$

(2) Discretize the PDE @ FDM

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{K^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{K^2} = H_{i,j}$$

$$u_{i,j} = \frac{1}{4}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} \right]$$ -- laplace

No. of Interior nodes $\rightarrow (M-1)^2$



(3) Translate BCs into eqs.

$u_{i,0} = u_1$

$u_{0,j} = u_2$

$u_{i,M} = u_3$

$u_{M,j} = u_4$

} Boundary Nodes.

Corner nodes (take Average) :-

$$u_{0,0} = \frac{u_1 + u_2}{2}$$

$$u_{0,M} = \frac{u_2 + u_3}{2}$$

$$u_{M,0} = \frac{u_1 + u_4}{2} \qquad u_{M,M} = \frac{u_3 + u_4}{2}$$

(4) Algebraic Equations :- interior points ↓ Boundary points ↓

Total no. :- $(M-1)^2 + 4(M-1) + 4$ ← corner points.

↳ $(M+1)^2$

Ex :- $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$

$0 \le x \le 1$

$0 \le y \le 1$

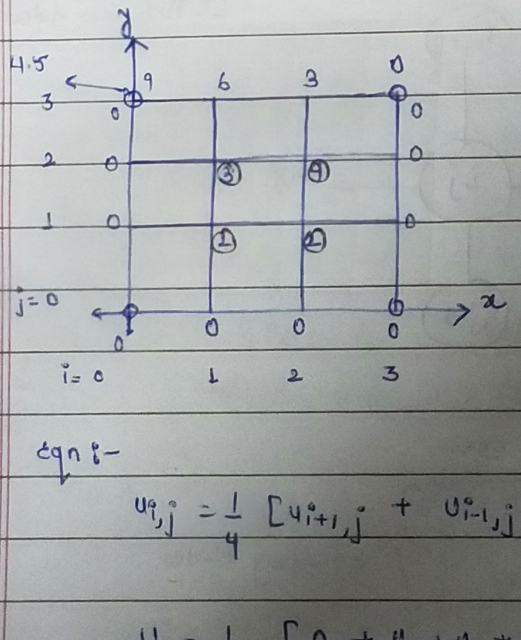
$M = 3$

$u(x,0) = 0$

$u(0,y) = 0$

$u(x,1) = 9(1-x)$

$u(1,y) = 0$



⊕→ position

eqn :-

$$u_{i,j} = \frac{1}{4}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right]$$ --- from previous general soln.

$$U_1 = \frac{1}{4}\left[0 + U_2 + U_3 + 0\right]$$

$$U_2 = \frac{1}{4}\left[U_1 + 0 + 0 + U_4\right]$$

$$U_3 = \frac{1}{4}\left[0 + 6 + U_4 + U_1\right]$$

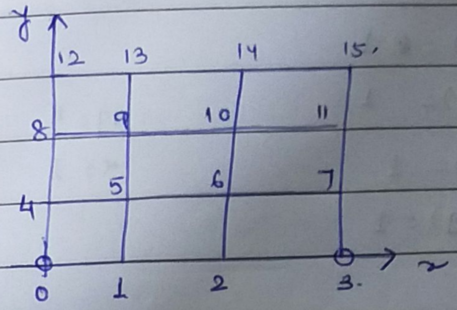
$$U_4 = \frac{1}{4}\left[3 + 0 + U_2 + U_3\right]$$

↳ Solve.

$M^2 - 2M + 2$

Revisit Step 2 :- (Discretize PDE)

instead of 2 indices (i, j)
if we use a Global index



global index (m)

$$m = i + j(M+1)$$

$i = 1,\ j = 1 \quad \Rightarrow \quad m = 5$

$i = 3,\ j = 2 \quad \Rightarrow \quad m = 11$

$i = M,\ j = M \quad \Rightarrow \quad m = M^2 + 2M$

∴ Discretize Equation :-

Step ① : $\quad k = 1/3$

Central difference,

Step (ii) :-
$$\frac{u_{m+1} - 2u_m + u_{m-1}}{k^2} + \frac{u_{m+M-1} - 2u_m + u_{m-(M+1)}}{k^2} = 0$$

$$u_{m+1} - 4u_m + u_{m-1} + u_{m+(M+1)} + u_{m-(M+1)} = 0.$$

Step ③ :- B : $u_m = u_1 \quad j = 0 \quad i = 0, 1, 2, M$

Bottom

$0 \le m \le M$

L : $u_m = u_2 \quad i = 0 \quad j = 0, 1, 2, - M$

left

$0 \le m \le M^2 + M$

('m' that lies on the left boundary only.)

T : $u_m = u_3 \quad i = 0, 1, 2, M \quad j = 3$

$- M^2 + M \le m \le M^2 + 2M$

$M \le m \le M^2 + 2M$

R : $U_m = U_y$

Ex:- $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \alpha u^2 = 0$

$u(x,0) = 1$

$u(0,y) = 1$

$u(x,1) = 1$

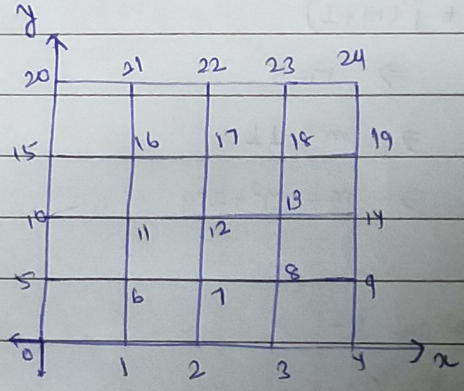
$u(1,y) = 1$

$M = 4$

$\alpha = 1$

$\Rightarrow U_{m+1} - 4U_m + U_{m-1} + U_{m+M+1} + U_{m-(M+1)} - k^2\alpha U_m^2 = 0 = g_m$

↳ Non-Linear eqn
(Solve by N-R)



m = 6, 7, 8

m = 11, 12, 13

m = 16, 17, 18.

$\cancel{g^{k+1}} = \cancel{g^k}$

$$U^{n+1} = U^n - (J^n)^{-1} G^n$$

$U = [\,U_6 \quad U_7 \quad U_8 \quad U_{11} \quad U_{12} \quad U_{13} \quad U_{16} \quad U_{17} \quad U_{18}\,]^T$

J = 9x9 matrix.