ODE Distillation Column (ODE IVP) 27/2/19

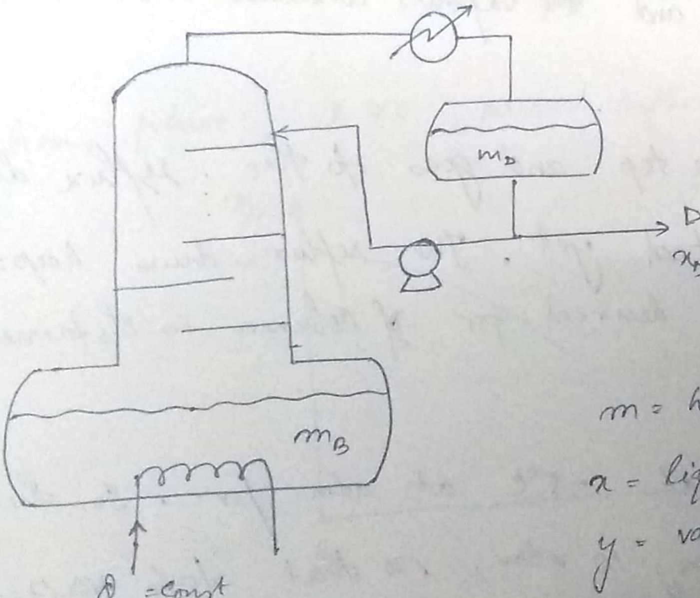
41431

Batch Distillation

In Continuous Distill. to separate N_c no. of components.

1. In continuous distill. column, to separate N_c components, $N_c - 1$ columns are needed. But in Batch Distil. Column, 1 column is enough.

2. Flexibility of batch column is more than continuous. Product comp. can be varied in batch distill. ~~col.~~ column.



m = holdup, liquid (mol)

x = liq. comp

y = vap. comp

L = Liq flow rate mol/time

V = vap flow rate mol/time

3. Batch distill. is an unsteady state process unlike continuous distill.

m_B is high for batch distill. than that for continuous distill. as the ~~feed~~ fresh feed is entered into the reboiler.

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Startup Phase: We can either enter the feed only to reboiler, or enter from top, so that all the trays as well as reboiler.

① Feed is entered only in the reboiler from feed tank

② Q is added in reboiler. $Q = m C_p \Delta T$ which is the sensible heat required to bring the liquid feed to saturation.

③ The vapours go up by a pressure driven force. Bottom has max. pr. and top has lowest pr.

④ As we go up, T ↓ and the vapours condense and collect in the trays.

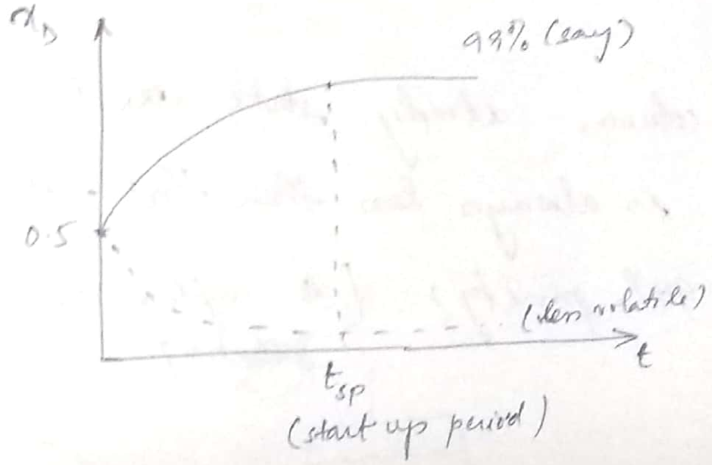
⑤ The vapour leaves the top and goes to the reflux drum. Condenser is not started yet. The reflux drum keeps filling with vap. until the desired pr. of column is obtained. Then condenser is started.

⑥ Some HC vaporize at −5°C at atm. pr. So, the pr. is increased to, say 10 atm, so that top vap. is at say 30°C, so that cheap coolant (water) can be used. At −5°C vap., refrigerator reqd is needed which is very expensive. So, we need to do cost calc. b/w reboiler heat duty, pr. and refrigeration cost

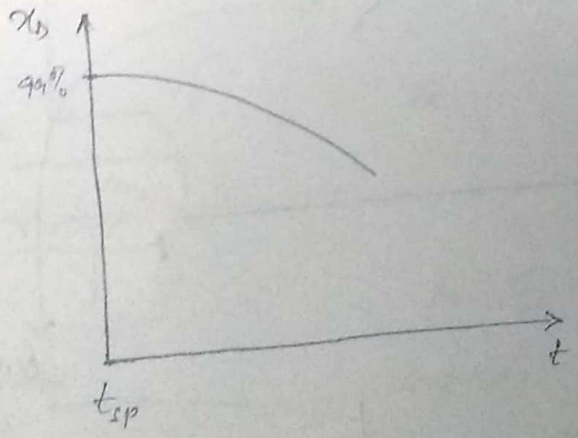
⑦ We give total reflux. Whatever is condensed is refluxed. called Total Reflux Operation. In reality, there is a time difference b/w condensation time and reflux transport time.

In the startup phase, $D = 0$

If the startup phase goes on, i.e. total reflux goes on, the column reaches steady state at max achievable product purity



Production phase: $D \neq 0$, partial reflux

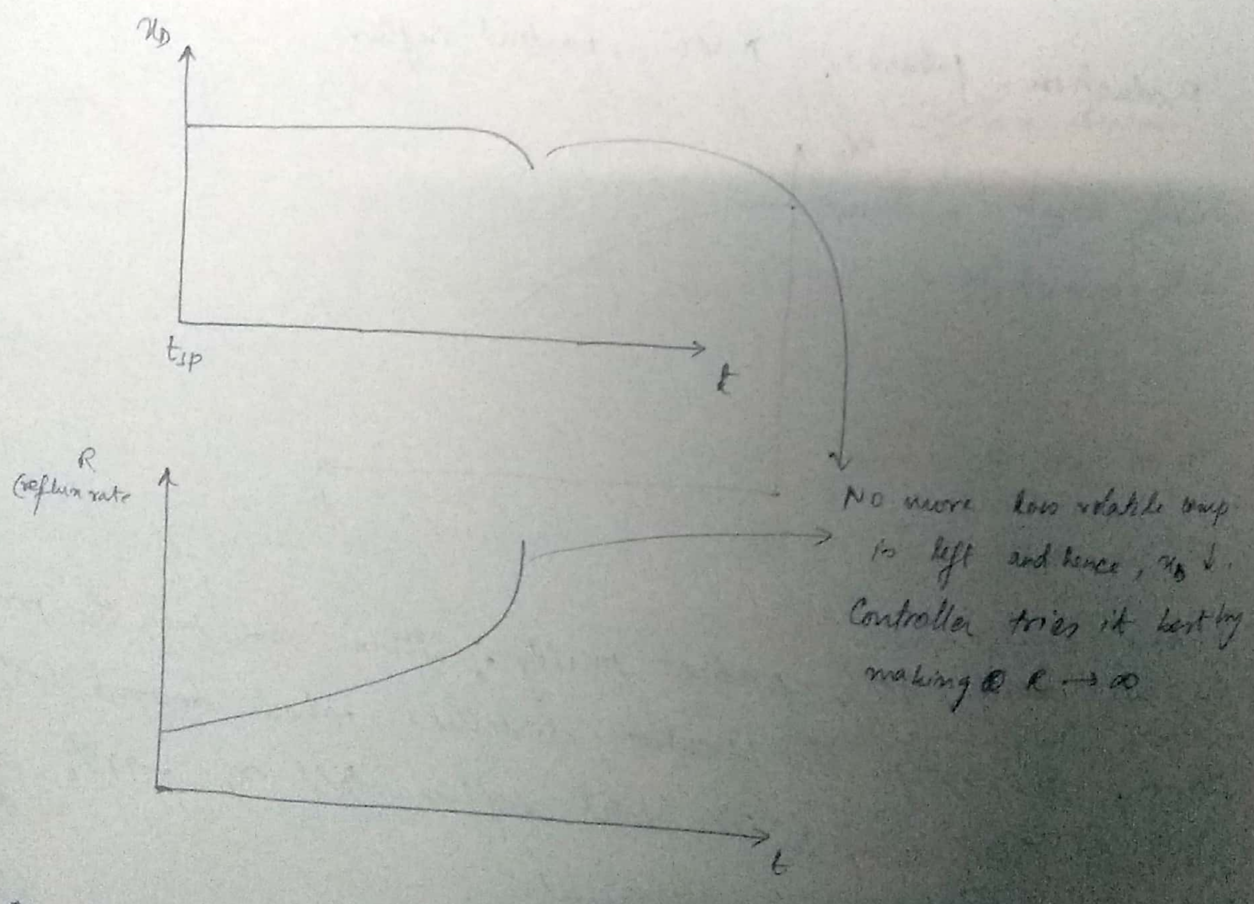


Say we want 95% product purity. Then, we run the production phase, and stop the ~~product~~ distillate when ~~desired~~ 95% is reached (avg. comp.). The total reflux till $x_D = 99\%$, again to start distillate withdrawal.

As reflux ~~ratio~~ rate ↑, product purity increases. During production phase, reflux is less than total reflux, so $x_D \downarrow$

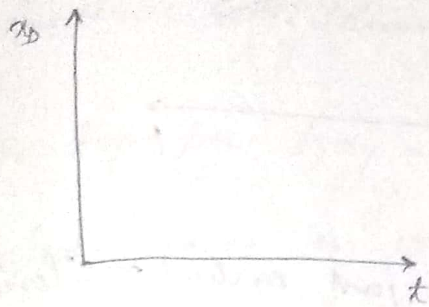
5. Say ~~R~~ R = 10 mol/min. If the pump goes out of, the replacement takes ~~10m~~ 10–15 min, so, the reflux drum should be capable of ~~holding~~ holding ~ 100 mol.

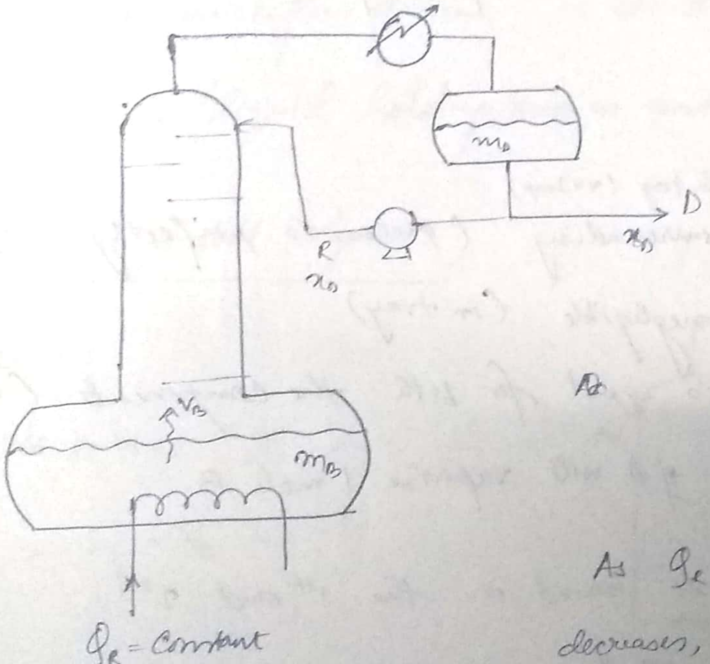
Q) In a batch column, steady state x_D is 99%. But product comp is always less than that. How do we get product at 99% purity? [As reflux rate ↓, x_D ↓ during production]



As we start taking out D, ~~m_B~~ m_D remains constant, but m_B ↓;

Batch Distillation (Continuation) 28/2/17





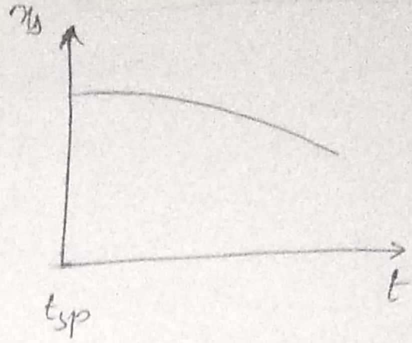
As Q_R is constant and m_B decreases, ∴ rate of evaporation increases. But m_B becomes more heavy. So, vaporization rate of boiler may not increase.

We basically want to increase the reflux rate to be more than total reflux at start up period.

When we use a controller a ± 5% level change is considered to be steady for a level controller. So, if the reflux drum size is large, the 5% can be taken out from reflux drum so that ... obtained at highest purity

5) ## Modes of Batch Distillation ~~(already discussed)~~

- Constant Reflux Ratio
  (Open loop)



- Constant Composition (discussed just earlier) — Closed loop

- Constant Distillate Rate — Open loop

Assumptions

- Perfect mixing in each tray (VVImp)
- No heat loss to surrounding (process is perfectly insulated)
- Vapour hold up is negligible (in tray)
- Heat of vaporization is equal for both the components (McCabe-Thiele Assumption)

One mole condensation of A will vaporise 1 mole B.

The 3rd assumption is based on the 1st and 2nd.

If there is heat loss, so then no equimolar counter diff

(3rd)

The vap. hold up is negligible as $\rho_{vap} \ll \rho_{liq}$.

But this is not true when there is high pr (close to critical pt)

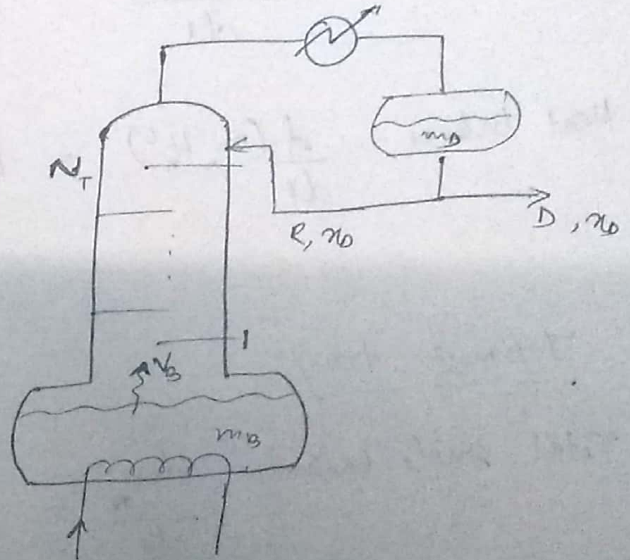
- Liquid hold up is variable (moles, not volume)
- Inefficient trays (include tray efficiency, $\eta = 70\%$ say)

If $\eta = 100\%$, then we have ideal distillation column

- We also have ideal distill. column when vap and liquid are ideal

- Liquid is non-ideal (activity coeffient, modified Raoult's law)
- Column pr. = 1 atm (say) → This is the top most pr.
  ↓
  Atmospheric Distil. Column
- Pr. drop per tray = 0.5 kPa (say)
- Perfect mixing in tray (no spatial variation of x in tray).
- Neglect coolant dynamics in condenser and heating dynamics in heat reboiler.
- Liquid holdup in reflux drum is constant due to controller.
- Tray volumetric liquid holdup remains constant

Modelling the Distill. column



① Reboiler

Total Mole balance :

$$\frac{dm_B}{dt} = L_1 - V_B = -D$$

- Component balance :

$$\frac{d(x_B m_B)}{dt} = L_1 x_1 - V_B y_B$$

Energy :

$$q_R = V_B \lambda$$ (neglecting thermal dynamics, assumed)

Or

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

② Bottom tray:

Total mole balance: $\frac{dm_1}{dt} = L_2 + V_B - L_1 - V_1$

Comp. balance: $\frac{d(m_1 x_1)}{dt} = \cancel{L_2 y_2} + L_2 x_2 + V_B y_B - L_1 x_1 - V_1 y_1$

Heat balance: $\frac{d}{dt}(m_1 H_1^L) = L_2 H_2^L + V_B H_B^V - L_1 H_1^L - V_1 H_1^V$

③ n-th tray:

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

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

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

④ Topmost tray:

Total mole balance: $\frac{dm_N}{dt} = R + V_{N-1} - L_N - V_N$

Comp. balance: $\frac{d(m_N x_N)}{dt} = R x_D + V_{N-1} y_{N-1} - L_N x_N - V_N y_N$

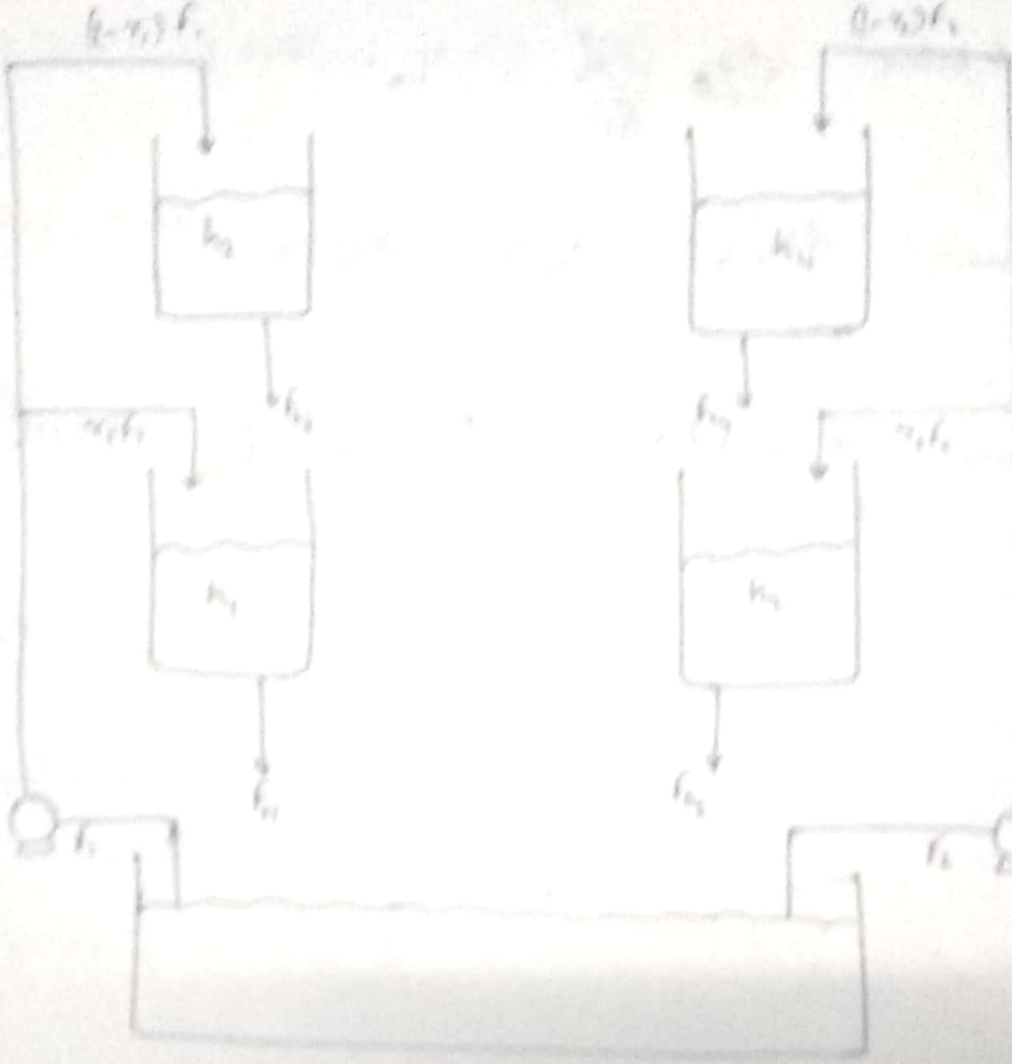
Heat balance: $\frac{d}{dt}(m_N H_N^L) = R H_R + V_{N-1} H_{N-1}^V - L_N H_N^L - V_N H_N^V$

Reflux drum

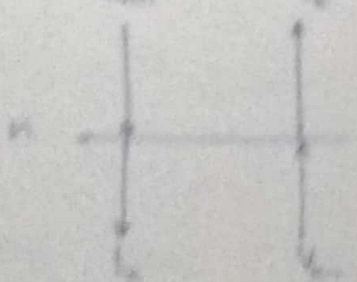
Total mole balance: $\frac{d\cancel{m_D}^{\,0}}{dt} = V_{N} - (R+D)$

Comp. balance: $\frac{d(m_D x_D)}{dt} = V_N y_N - (R+D)\, x_D$

Heat Balance: $\frac{d}{dt}(m_D H_D^L) = \cancel{V_N H_N} \; V_N H_N^V + q_{condenser} - (R+D)\, H_D^L$



Distillation ([illegible])



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

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

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

We are not considering McCabe Thiele, so V is variable.

Variables

m ~~(mol)~~ , ~~x (mol fraction~~
(holdups)

m (mol) . . . . from Total Mole Balance
(outlet holdups)

x (mol fraction) . . . . Component Balance

T (as enthalpy of pure comp is $f(T)$) . . . . . Bubble Pt Calculation

y (mol fraction)

L (mol/min)

V (mol/min)

Vapour Liquid Eqm.

T calculation: ~~Raoult's~~ Raoult's law: $P_i = P_i^\circ x_i$ . . . ideal (L)

Dalton's Law: $P_i = P_t \cdot y_i$ . . . ideal (V)

$$\therefore P_i^\circ x_i = P_t y_i$$

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

k_i: VLE coeff

$$\text{Relative volatility} = \alpha_{ij} = \frac{k_i}{k_j} = f(T, P_t)$$

If we assume constant α_{ij} then we assume constant T throughout the column which is not true.

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$$\therefore y_i = k_i x_i$$

$$\Rightarrow k_i = \frac{y_i}{x_i}$$

$$k_j = \frac{y_j}{x_j} = \frac{(1-y_i)}{(1-x_i)}$$

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

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

Case 1: 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

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

$$y_2 = 1 - y_1$$

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1. Assume T
2. Find P_i^o (Antoinne eq^n)
3. $\gamma_i = f(T, x_i)$
4. $y_i = \dfrac{P_i^o x_i \gamma_i}{P_t}$
5. Convergence $|\Sigma y_i - 1| \leq tol.$
6. $f(T) = \Sigma y_i - 1$
7. $T_{new} = T_{old} - \dfrac{f(T)}{f'(T)}$

For only liq. phase non-ideality : $\gamma_i P_i^o x_i = P_t y_i \Rightarrow k_i = \dfrac{\gamma_i P_i^o}{P_t}$

For liq. + vap. non-ideality : $k_i = \dfrac{\hat{f}_i^L / P_t x_i}{\hat{f}_i^V / P_t y_i}$

ϕ = fugacity

find from eq^n of state (like Peng Robinson, RK, SRK etc)

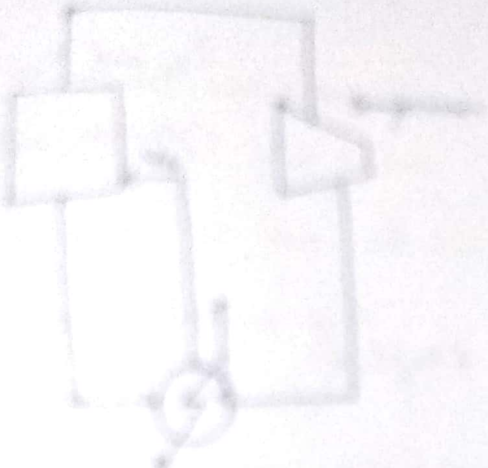
One approach to find k_i is $\gamma - \phi$ — heterogeneous

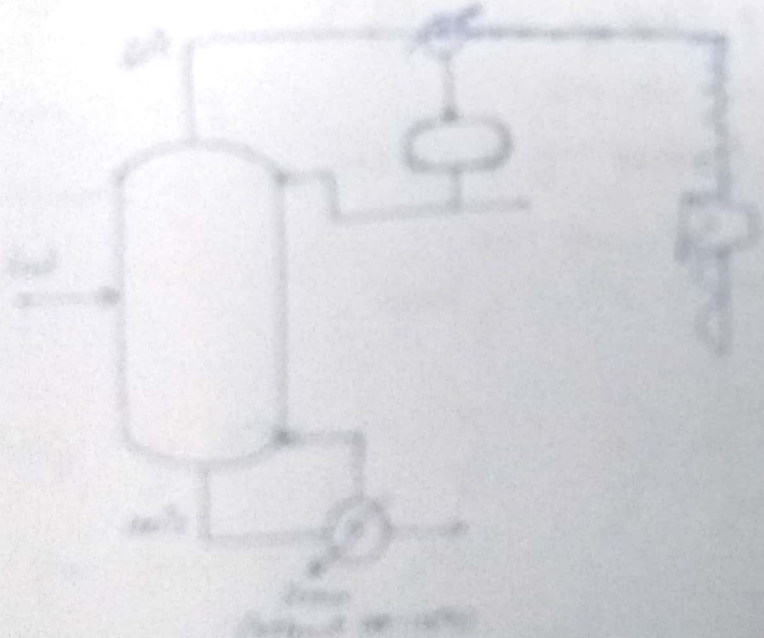
$\phi_L - \phi_v$ — homogeneous

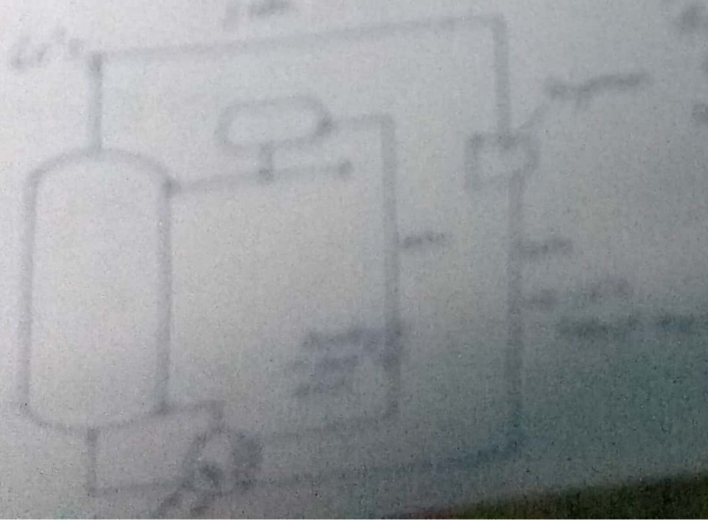
In case of tray temp. , we assume $T_L = T_V$ (thermal eq^m)

But in reality, there is some difference b/w liq. and vap. phase temp. as vaporization at bubble pt. and condensation at dew pt.

For binary mix., dew pt. and bubble pt. temp. are different







5 Flow rate (L)

Francis - Weir Eqⁿ

$$L_n = L_{n0} + \frac{M_n - M_{n0}}{\beta}$$

L_{n0} and M_{n0} are reference values

Above feed tray, $L_{n0} = R$ (reflux)

Below feed tray, $L_{n0} = F + R$

m_{n0} is taken as 0 (hold up initially).

β = hydraulic time constant, 3 - 6 sec.

Distillation Column (Continuation)

7/3/19

Variable list :

m — Total mole balance

x — Component mole balance

y — Bubble pt temp. calculation

V — Energy Balance Eq^n

δL — Francis-Weir Eq^n

T — Bubble Pt. temp calculation

Vapour Liquid Equilibrium

Known : x, P_t

Unknown : y, T

From this calculation, the y we get is eqm. y, i.e. $y = y^*$.

But trays are not ideal so, how to get the actual y? Here we need to consider tray efficiency.

Murphy Tray Efficiency : $\eta = \dfrac{y_n - y_{n-1}}{y_n^* - y_{n-1}}$

Point efficiency
Tray efficiency
Column efficiency

$\Rightarrow y_n = y_{n-1} + \eta (y_n^* - y_{n-1})$

y_n^* we get from Bubble Pt calculation

How to get y_{n-1} ? Condenser and reboiler we have $y = y^*$ if they are 100% efficient

If we start from reboiler, y_B is known

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

for subsequent y_2, y_1 is known, for y_3, y_2 is known, etc.

5. How to calculate the enthalpy?

<u>Enthalpy</u>

We need to know the temp. T, pr. P and composition

For vapour phase, the eq^n. used is :

* H_v is for a particular component

$$H^V = \int_{T_0}^{T} C_p \, dT \quad , \quad T_0 = \text{ref. temp}$$

C_p expr. for diff. components are available in data books

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

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

or, $$H^V = \sum_{k=1}^{n} \frac{a_k (T^k - T_0^k)}{k}$$

If T_0 changes, $a_1, a_2, \ldots$ values change.

Case 1: $T_0 = 0$ (Henley & Seader)

$$\therefore H^V = \sum_{k=1}^{n} \frac{a_k T^k}{k} \quad , \; a_k \text{ values available}$$

Case 2: $T_0 = 25^\circ C$

, a_k values available

Book

* Henley and ~~Staden~~ Seader

* Properties of gas and liquids

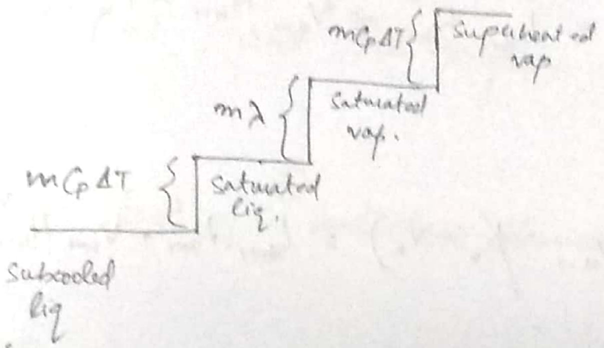
* Prausnitz

values are available component wise.

$$H^v_{total} = \sum_i H_{v_i} y_i$$

How to calculate enthalpy for liquid component ?

We just subtract the latent heat of vap. of that component from H^V_i



Liquid Enthalpy :

$\therefore$ ~~Ho~~ $H_i^L = H_i^V - \lambda_i$ for a component

$H^L = H^V - \lambda$ for a stream

We can calculate λ from Clausius-Clapeyron Eq^n :

$$\frac{d(\ln P^\circ)}{dT} = \frac{\lambda}{RT^2} \longrightarrow \text{Clausius Clapeyron Eq}^n$$

$$\ln P^\circ = A - \frac{B}{T+C} \longrightarrow \text{Antoinne Eq}^n.$$

Substituting,

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

So, we can calculate the enthalpy of liquid H^L_i and H^L

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Vapour flow rate

Energy Balance eq^n for n^th tray

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

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

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

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

It requires H_n^L value at $t+1$. So, we need to use iterative method.

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

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

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

Iterative method

Let's assume, at $t = t$, $V_n = V_{n_0}$.

① Assume V_n at time t.

② Compute x_n at $t+1$ from Component Balance eq^n.

③ Bubble pt. temp. computation at $t = t+1$, i.e. T @ $t+1$.

④ Calculate H_n^L at $t+1$, and then compute $\frac{dH_n^L}{dt} = \frac{H_n^L(t+1) - H_n^L(t)}{\Delta t}$

⑤ Calculate V from last eq^n ④ ~~and check the convergence~~

⑥ Check Convergence.

⑦ If not converging, go to step ② and use the V_n value calculated from eq^n ④.

The exact ways are:

(I) $\frac{d}{dt}(m_n H_n^L) = 0 = L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - L_n H_n^L - V_n H_n^V$

(II) $H_n^L \frac{dm_n}{dt} + 0 = L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - L_n H_n^L - V_n H_n^V$

Assignment

Simulate the entire distillation Column

5

Midsem 8/3/19

Q 2a) Bubble Pt Calculation.

$P_i = P_i^s x_i$ --- Roult's Law

$P_i = P_t y_i$ --- Dalton's law

$y_i = k_i x_i = \frac{P_i^s}{P_t} x_i$

$\Rightarrow k_i = \frac{P_i^s}{P_t}$

$y_1 = k_1 x_1$

$1 - y_1 = k_2 (1 - x_1)$

$1 = k_1 x_1 + k_2 (1 - x_1)$

$\Rightarrow x_1 = \frac{1 - k_2}{k_1 - k_2} = \frac{P_t - P_2^s}{P_1^s - P_2^s}$

1. Assume a T_0.
2. Find x_1 and x_2
3. Find y_1 and y_2
4. Check $|\Sigma y_i - 1| \leq tol$
5. Take $f(T) = \Sigma y_i - 1$
6. $T_{k+1} = T_k - \frac{f(T_k)}{f'(T_k)}$

But no. of variables is 3 (x, y, T) and eq^ns are 2, so $f = 1$. So if we take any T, it'll give some x, y.

From

Simu

① Inp

② As

③ Q_R

Reboiler Heat Du

④ Bu

⑤ En

⑥ Lo

⑦

Pr

fe

⑦

⑧

⑨ To

From what we did for Distillation

Simulation Algorithm

1) Input specification:

- Feed (composition, flowrate (for continuous, not batch), quality)
- Column Dimension (diameter, weir dimensions), weir height ~ 2-4 in.)
  length ~ 80-85% of the column dia.
- Pressure profile
- Tray efficiency (η)
- Hydraulic Time constant (β in Francis-Weir formula).
- C_p coefficients

2) As it is an ODE-IVP Problem:

- Initialize : $m(0)$, $x(0)$, $T(0)$
  for Bubble Pt Calc.

3) Q_R & R
Reboiler Heat Duty
Reflux Rate

4) Bubble Point Temp Calculation ⇒ Calculate T, y^*, y (using η)

5) Enthalpy - As T, x_i, y_i are known

6) Liquid flow rate : $L_n = L_{n0} + \dfrac{m_n - m_{n0}}{\beta}$.

* Initial guess for m_n is $m_n = m_{n0}$
Provided feed is liquid, $L_{n0} = R$ above feed tray and $L_{n0} = R+F$ below feed tray

7) V_n

8) $m(t+1)$, $x(t+1)$

9) To continue the simulation, go back to step (3).

5

For B & D

B Total Mole Balance m_B } maintained constant by

D Total Mole Balance m_D } level controller.

g) $\frac{dx}{dt} = 5e^{-x^2}$ Implicit Euler

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

For initial value, use iterative method.

$$f(w) = w - x_k - 5h\exp(-w^2)$$

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

5

14/3/19

ODE - BVP

Dirichlet BC

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

$u(0) = 1$ $\qquad\qquad$ $u_4 = 0.138889$

$u(1) = 0$

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

$m = 1$:

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

$m = 2$

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

$m = 3$

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

$m = 4$

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

$m = 5$

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

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

$x^2\sqrt{2}.\ \exp\left(\frac{-x}{2}\right) = .97$

$u_1 = 0.138889$

$\Rightarrow u_2 = 2u_1 - 2h^2 = 2 \times 0.138889 - \frac{2}{6^2}$

$\Rightarrow u_2 = 0.222222$ — (i)

$u_3 = 2u_2 - u_1 - 2h^2$

$\Rightarrow u_3 = 0.249999$ — (ii)

$u_4 = 2u_3 - u_2 - 2h^2$

$\Rightarrow u_4 = 0.222220$ — (iii)

$u_5 = 2u_4 - u_3 - 2h^2$

$\Rightarrow u_5 = 0.138885$ — (iv)

$u_6 = 0$

Find analytical

x	Numerical	Analytical
0	0	
$\frac{1}{6}$	0.138889	
$\frac{2}{6}$	0.222222	
$\frac{3}{6}$	0.249999	
$\frac{4}{6}$	0.222220	
$\frac{5}{6}$	0.138885	
$\frac{6}{6}$ 1	0	

5.

Neumann BC

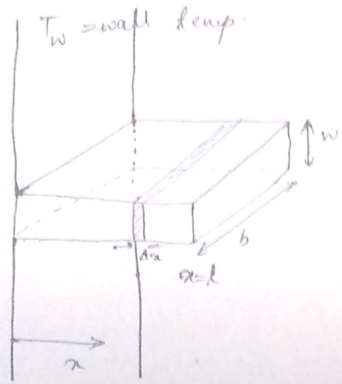
Fin Problem

$$\frac{d^2T}{dx^2} = \frac{hP}{kA}(T - T_0)$$

P = perimeter = 2(w+b)

A = conductive HT area

~~HT~~ Area for convective HT = $P\Delta x$



T_0 = ambient temp

$l = 4$

$$\frac{hP}{kA} = 1$$

BC: $T(x=0) = T_w$

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

$m = 4$

Ans:- Non-dimensionalizing :-

$$\theta = \frac{T - T_0}{T_w - T_0}$$

$$\xi = \frac{x}{l}$$

$$H = \sqrt{\frac{hPl}{kA/l}} = \sqrt{\frac{hPl^2}{kA}}$$

$\therefore \frac{(T_w - T_0)}{L^2}\frac{d^2\theta}{d\xi^2} = \frac{hP}{kA}\cancel{(T_w - T_0)}\,\theta$

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

BC: @ $\xi = 0$, $\theta = 1$ (Dirichlet BC)

@ $\xi = 1$, $\frac{\partial\theta}{\partial\xi} = 0$ (Neumann BC)

$m = 1$:

$k = \frac{\xi_m - \xi_0}{m}$

$= \frac{1}{4}$

$\cancel{T_2 + T_0 - 2T_1} = \cancel{\ \ } H^2 T_1$

$\theta_2 + \theta_0 - 2\theta_1 = H^2\theta_1 k^2 \quad \text{--- (1)}$

$m = 2$:

$\theta_3 + \theta_1 - 2\theta_2 = H^2\theta_2 k^2 \quad \text{--- (2)}$

$m = 3$

$\theta_4 + \theta_2 - 2\theta_3 = H^2\theta_3 k^2 \quad \text{--- (3)}$

$m = 4$

~~From Neumann BC:~~

$\theta_5 + \theta_3 - 2\theta_4 = H^2\theta_4 k^2 \quad \text{--- (4)}$

From Neuman BC: $\frac{\theta_5 - \theta_3}{2k} = 0$

$\Rightarrow \theta_5 = \theta_3 \quad \text{--- (5)}$

From (4) & (5),

$2\theta_3 - 2\theta_4 = H^2\theta_4 k^2$

$\Rightarrow 2\theta_3 = \theta_4(2 + H^2k^2) \quad \rightarrow \theta_3 = \frac{(2 + H^2k^2)}{2}\theta_4 \quad \text{--- (6)}$

$$\Rightarrow \theta_4 = \left(\frac{2}{2+H^2k^2}\right)\theta_3 \quad \text{--- (a)}$$

Putting in (3),

$$\left(\frac{2}{2+H^2k^2}\right)\theta_3 + \theta_2 - 2\theta_3 = H^2k^2\theta_3$$

$$\Rightarrow \theta_3\left(\frac{2}{2+H^2k^2} - 2 - H^2k^2\right) = -\theta_2$$

$$\Rightarrow \theta_3\left(\frac{2 - 4 - 2H^2K^2 - 2H^2k^2 - H^4k^4}{2+H^2k^2}\right) = -\theta_2$$

$$\Rightarrow \theta_3\left(\frac{2 + 4H^2k^2 + H^4k^4}{2+H^2k^2}\right) = \theta_2$$

$$\Rightarrow \theta_3 = \left(\frac{2+H^2k^2}{2+4H^2k^2+H^4k^4}\right)\theta_2 \quad \text{--- (b)}$$

~~putting in~~ (2)

$$H = l\sqrt{\frac{hP}{kA}} = 4$$

$$k = \frac{1}{4}$$

$$\theta_3 = \left(\frac{2+1}{2+4+1}\right)\theta_2 = \frac{3}{7}\theta_2 \quad \text{--- (b)}$$

Putting in (2)

$$\theta_3 + \theta_1 - 2\theta_2 = \theta_2 \Rightarrow \frac{3}{7}\theta_2 + \theta_1 - 3\theta_2 = 0$$

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

$\Rightarrow \theta_2 = \frac{7}{18}\theta_1$ —— ⓒ

Putting in ①

$\theta_2 + 1 - 2\theta_1 = \theta_1$

$\Rightarrow \frac{7}{18}\theta_1 + 1 - 3\theta_1 = 0$

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

$\Rightarrow \theta_1 = \frac{18}{47} = 0.38298$

$\theta_2 = 0.14894$

$\theta_3 = 0.06383$

$\theta_4 = \frac{2}{3} \times \theta_3 = 0.04255$

Analytical Solⁿ.

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

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

$\Rightarrow \theta = M_1 e^{-4\xi} + M_2 e^{4\xi}$

@ $\xi = 0$, $\theta = 1$

$\Rightarrow 1 = M_1 + M_2$ —— Ⓐ

@

5.

$$\frac{d\theta}{d\xi} = -4\left[M_1 e^{-4\xi} - M_2 e^{4\xi}\right]$$

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

$\therefore 0 = -4\left[M_1 e^{-4} - M_2 e^{4}\right]$

$\Rightarrow M_1 e^{-4} = M_2 e^{4}$

$\Rightarrow M_1 = e^{8} M_2 \quad \text{— (6)}$

$\therefore M_1 + M_2 = 1$

$\Rightarrow M_2(1 + e^{8}) = 1$

$\Rightarrow M_2 = 3.3535 \times 10^{-4}$

$\therefore M_1 = 0.999665$

$\therefore \theta = 0.999665\, e^{-4\xi} + 3.3535 \times 10^{-4}\, e^{4\xi}$

@ $\xi = 0$, $\theta = 1$

@ $\xi = \frac{1}{4}$, $\theta = 0.36867$

@ $\xi = \frac{2}{4}$, $\theta = 0.137768$

@ $\xi = \frac{3}{4}$, $\theta = 0.056506$

@ $\xi = 1$, $\theta = 0.03662$

$$\dots + z_0 - k^2 \left(z_2 \exp\left(\frac{-a}{z_0}\right)\right) = ?$$

Here, the deviation is more. So increase m.

15/3/19

Ex: An isothermal tubular reactor : Robin BC + Non-linear case

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

Pe = Peclet No. = 6

Da = Damkohler No. = 2

$x \in [0, 1]$

> The model eqⁿ is given in dimensionless form as dimensionless groups Pe & Da are there

BCs:

$$\left.\frac{dc}{dx}\right|_{x=0} = P_e (c-1) \quad \dots\dots \text{Robin B.C.}$$

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

Consider m = 6, and central finite diff. approximation

$k = \frac{1}{6}$.

Ans. ~~m=0~~

$$\frac{1}{Pe}\frac{d^2c}{dx^2} - \frac{dc}{dx} = Da \cdot c^2$$

$$\Rightarrow \frac{d^2c}{dx^2} - Pe \cdot \frac{dc}{dx} = Da \cdot Pe \, c^2$$

$$\Rightarrow \frac{d^2c}{dx^2} - 6\frac{dc}{dx} = 12 c^2$$

$$\Rightarrow \frac{C_{m+1} - 2C_m + C_{m-1}}{k^2} - 6\left(\frac{C_{m+1} - C_{m-1}}{2k}\right) = 12 C_m^2$$

$$\Rightarrow C_{m+1} - 2C_m + C_{m-1} - 3k\,(C_{m+1} - C_{m-1}) = 12k^2 C_m^2$$

$$\Rightarrow (1-3k)\,C_{m+1} - 2C_m + (1+3k)\,C_{m-1} = 12k^2 C_m^2$$

$$\Rightarrow \frac{1}{2} C_{m+1} - 2C_m + \frac{3}{2} C_{m-1} = 12k^2 C_m^2$$

$$\Rightarrow C_{m+1} - 4C_m + 3C_{m-1} = \cancel{24k^2}\ \frac{2}{3} C_m^2$$

5 $\Rightarrow C_{m+1} = \frac{2}{3} C_m^2 + 4C_m - 3C_{m-1}$ ← ⊛

$\underline{m=0}$

$C_1 = \frac{2}{3} C_0^2 + 4C_0 - 3C_{-1}$ ← (i)

$\underline{m=1}$

$C_2 = \frac{2}{3} C_1^2 + 4C_1 - 3C_0$ ← (ii)

$\underline{m=2}$

$C_3 = \frac{2}{3} C_2^2 + 4C_2 - 3C_1$ ← (iii)

$\underline{m=3}$

$C_4 = \frac{2}{3} C_3^2 + 4C_3 - 3C_2$ ← (iv)

$\underline{m=4}$

$C_5 = \frac{2}{3} C_4^2 + 4C_4 - 3C_3$ ← (v)

$\underline{m=5}$

$C_6 = \frac{2}{3} C_5^2 + 4C_5 - 3C_4$ ← (vi)

$\underline{m=6}$

$C_7 = \frac{2}{3} C_6^2 + 4C_6 - 3C_5$ ← (vii)

$\frac{C_1 - C_{-1}}{2h} = Pe\,(C_0 - 1)$ ... Robin BC

$\Rightarrow C_{-1} = C_1 - 2h\,Pe\,(C_0 - 1)$

$\Rightarrow C_{-1} = C_1 - 2(C_0 - 1)$ ← (viii)

$$\cdots + z_0 - k^2 \gamma z_2 \exp\left(\frac{-\alpha}{z_1}\right) = g_7$$

$$\frac{C_7 - C_5}{2h} = 0 \quad \text{--- Neumann BC}$$

$\Rightarrow C_7 = C_5$ —— (ix)

~~Putting (ix) in (vii)~~ Putting (ix) in (vii):

$C_5 = \frac{2}{3} C_6^2 + 4C_6 - 3C_5 \Rightarrow -12C_6 + 12C_5 = 2C_6^2$ —— (vii)

$\cancel{C_5 = \frac{2}{3} C_6^2 + 4C_6 - 3C_5}$

$\because$ We get non-linear eq^n, we have to use N-R in matrix form.

Substituting (viii) in (i)

$$C_1 = \frac{2}{3} C_0^2 + 4C_0 - 3[C_1 - 2C_0 + 2]$$

$$\Rightarrow C_1 = \frac{2}{3} C_0^2 + 4C_0 - 3C_1 + 6C_0 - 6$$

$$\Rightarrow 4C_1 = \frac{2}{3} C_0^2 + 10C_0 - 6$$

$$\Rightarrow 12C_1 = 2C_0^2 + 30C_0 - 18$$

$$\Rightarrow 12C_1 - 30C_0 = 2C_0^2 - 18 \quad \text{—— (i)}$$

General eq^n

$$C_{m+1} - 4C_m + 3C_{m-1} = \frac{2}{3} C_m^2 \quad \text{—— (A)} \Rightarrow 3C_{m+1} - 12C_m + 9C_{m-1} = 2C_m^2$$

$$\begin{bmatrix} -30 & 12 & 0 & 0 & 0 & 0 & 0 \\ 9 & -12 & 3 & 0 & 0 & 0 & 0 \\ 0 & 9 & -12 & 3 & 0 & 0 & 0 \\ 0 & 0 & 9 & -12 & 3 & 0 & 0 \\ 0 & 0 & 0 & 9 & -12 & 3 & 0 \\ 0 & 0 & 0 & 0 & 9 & -12 & 3 \\ 0 & 0 & 0 & 0 & 0 & 12 & -12 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \vdots \\ \vdots \\ C_6 \end{bmatrix} = \begin{bmatrix} 2C_0^2 - 18 \\ 2C_1^2 \\ \vdots \\ \vdots \\ 2C_6^2 \end{bmatrix}$$

5)

$$-30C_0 + 12C_1 = 2C_0^2 - 18 \quad \text{— (i)}$$

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

$$F = \begin{bmatrix} -30C_0 + 12C_1 - 2C_0^2 + 18 \\ 9C_0 - 12C_1 + 3C_2 - 2C_1^2 \\ 9C_1 - 12C_2 + 3C_3 - 2C_2^2 \\ 9C_2 - 12C_3 + 3C_4 - 2C_3^2 \\ 9C_3 - 12C_4 + 3C_5 - 2C_4^2 \\ 9C_4 - 12C_5 + 3C_6 - 2C_5^2 \\ 12C_5 - 12C_6 - 2C_6^2 \end{bmatrix};
\quad
J = \begin{bmatrix} -30-2C_0 & 12 & 0 & 0 & 0 & 0 & 0 \\ 9 & -12-2C_1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 9 & -12-2C_2 & 3 & 0 & 0 & 0 \\ 0 & 0 & 9 & -12-2C_3 & 3 & 0 & 0 \\ 0 & 0 & 0 & 9 & -12-2C_4 & 3 & 0 \\ 0 & 0 & 0 & 0 & 9 & -12-2C_5 & 3 \\ 0 & 0 & 0 & 0 & 0 & 12 & -12-4C_6 \end{bmatrix}$$

$$X = \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \end{bmatrix}$$

Initial guess $\Rightarrow$ All 0

$$X_{n+1} = X_n - J^{-1} F$$

Final Answer

$C_0 = 0.83009$

$C_1 = 0.69007$

$C_2 = 0.58748$

$C_3 = 0.50978$

$C_4 = 0.44993$

$C_5 = 0.40535$

$C_6 = 0.38114$

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$\ldots + z_8 - k^2 r z_2 \exp\left(-\frac{\alpha}{z_7}\right) = g_7$

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

BC: $a_0 y(a) + b_0 y'(a) = C_0$ ... Robin BC

$a_1 y(b) + b_1 y'(b) = C_1$ ... Robin BC

Solve in general terms for m points.

Ans: 1st BC: (Left boundary)

$$y(x+k) = y(x) + \left(\frac{dy}{dx}\right)k + \frac{1}{2}\left(\frac{d^2y}{dx^2}\right)k^2 + \cdots$$

$$y(x+2k) = y(x) + \left(\frac{dy}{dx}\right)2k + \frac{1}{2}\left(\frac{d^2y}{dx^2}\right)4k^2 + \cdots$$

$$y(x+2k) - 4y(x+k) = \left[y(x) + 2k\,y'(x) + \frac{4k^2}{\cancel{2}}\,y''(x) + \cdots\right]$$
$$- 4\left[y(x) + k\,y'(x) + \frac{k^2}{2}\,y''(x) + \cdots\right]$$
$$= -3y(x) - 2k\,y'(x) + O(k^3)$$

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

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

Here, we won't get fictitious value of y_{-1} for y_0'

$$y_0' = y'(a) = \frac{-3y_0 + 4y_1 - y_2}{2k}$$

Right Boundary

$$y(x-k) = y(x) - k y'(x) + \frac{k^2}{2} y''(x) - \cdots$$

$$y(x-2k) = y(x) - 2k y'(x) + \frac{4k^2}{2} y''(x) - \cdots$$

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

~~$\Rightarrow y'(x) = 3y(x$~~

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

$$\therefore y_M' = \frac{3y_M - 4y_{M-1} + y_{M-2}}{2k}$$

$\therefore$ BC1: $a_0 y_0 + b_0 y_0' = C_0$

$$\Rightarrow a_0 y_0 + b_0 \left[\frac{-3y_0 + 4y_1 - y_2}{2k}\right] = C_0$$

$$\Rightarrow \left(a_0 - \frac{3b_0}{2k}\right) y_0 + \frac{2b_0}{k} y_1 - \frac{b_0}{2k} y_2 = C_2 \quad \cdots \quad \text{(BC1)}$$

$$\cdots + z_8 - k^2 \sqrt{z_2}\, \exp\left(-\frac{\alpha}{z_7}\right) = g_7$$

BC2: $a_1 y_M + b_1 y_M' = C_1$

$$\Rightarrow a_1 y_M + b_1 \left[\frac{3y_M - 4y_{M-1} + y_{M-2}}{2h}\right] = C_1$$

$$\Rightarrow \left(a_1 + \frac{3b_1}{2h}\right) y_M - \frac{2b_1}{h} y_{M-1} + \frac{b_1}{2h} y_{M-2} = C_1 \quad \text{--- } \{m = M\} \text{ (BC2)}$$

The discretize the modelling eq^n. using Central difference approximation and take m from 1 to $(M-1)$.

So, we can express the $(M+1)$ eq^{n}s [2 BC and $(M-1)$ modelling eq^n] in matrix form and solve.

5

20/3/19

Cooling Fin System

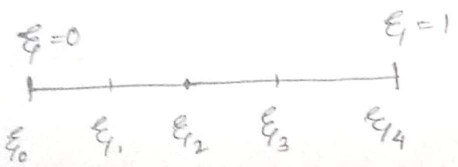
From last class

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

$$\theta(0) = 1$$

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

$M = 4$



ξ	Analytical	Numerical
0	1	1
0.25	0.3687	0.3830
0.5	0.1378	0.1489
0.75	0.0565	0.0638
1	0.0366	0.0425

The mismatch can be reduced by

(1) Mesh Refinement, i.e. increase M → no. of intervals

One way

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

Here, $M = 8$ $M = 4$

(2) In the ~~Dirichlet~~ Neumann Boundary condition, we can avoid using the fictitious pt. of ξ_5

for M=8 $\exp\left(\frac{-\alpha}{2}\right)$ = g7

ξ	Analytical	Numerical
0	1	1
0.125	0.60688	0.6100
0.25	0.3687	0.3725
0.375	0.22456	0.2281
0.5	0.1378	0.1407
0.625	0.086143	0.0885
0.75	0.0565	0.0584
0.875	0.041293	0.0429
1	0.0366	0.0381

$$\theta = 0.999665\, e^{-4\xi} + 3.3535\times10^{-4}\, e^{4\xi}.$$

(2) For avoiding the fictitious term, we can use forward diff. at $\xi=0$ and backward diff. at $\xi=1$, but they are 1st order accurate. So, we use central diff. is 2nd order accurate, and central diff. which is 2nd order use the formula derived in last class

$$\theta_{m-1} - 3\theta_m + \theta_{m+1} = 0$$ (Governing eq^n) (from m = 1 to m=3)

BC: $$\theta_M' = \frac{3\theta_M - 4\theta_{M-1} + \theta_{M-2}}{2k}$$

$\theta = 1$

5

$m=1$

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

$\Rightarrow 1 - 3\theta_1 + \theta_2 = 0 \quad \text{--- (i)}$

$m=2$

$\theta_1 - 3\theta_2 + \theta_3 = 0 \quad \text{--- (ii)}$

$m=3$

$\theta_2 - 3\theta_3 + \theta_4 = 0 \quad \text{--- (iii)}$

$$\theta_4' = 1 = \frac{3\theta_4 - 4\theta_3 + \theta_2}{2k} \quad \text{--- (iv)} \qquad k = \frac{1}{4}$$

$\Rightarrow 3\theta_4 - 4\theta_3 + \theta_2 = \frac{1}{2} \quad \text{--- (iv)}$

$$\begin{bmatrix} -3 & 1 & 0 & 0 \\ 1 & -3 & 1 & 0 \\ 0 & 1 & -3 & 1 \\ 0 & 1 & -4 & 3 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{2} \end{bmatrix}$$

From (iii), $\theta_2 = 3\theta_3 - \theta_4 \quad \text{--- (a)}$

Putting in (iv), $3\theta_4 - 4\theta_3 + 3\theta_3 - \theta_4 = \frac{1}{2}$

$\Rightarrow 2\theta_4 - \theta_3 = \frac{1}{2} \quad \text{--- (b)}$

$\therefore \theta_2 = 3\theta_3 - \frac{1}{2}\left(\theta_3 + \frac{1}{2}\right) = \frac{5}{2}\theta_3 - \frac{1}{4}$

$\Rightarrow \theta_3 = \frac{2}{5}\left(\theta_2 + \frac{1}{4}\right) \quad \text{--- (c)}$

Putting in (ii)

$\theta_1 - 3\theta_2 +$

Putting in (1)

$$\theta_1 - 3\theta_2 + \frac{2}{5}\left(\theta_2 + \frac{1}{4}\right) = 0$$

$$\Rightarrow \theta_1 - 3\theta_2 + \frac{2}{5}\theta_2 + \frac{1}{10} = 0$$

$$\Rightarrow \theta_1 = \frac{13}{5}\theta_2 - \frac{1}{10} \quad \Rightarrow \frac{5}{13}\left(\theta_1 + \frac{1}{10}\right) = \theta_2 \quad — (4)$$

Putting in (1),

$$1 - 3\theta_1 + \frac{5}{3}\left(\theta_1 + \frac{1}{10}\right) = 0$$

$$\Rightarrow 1 = \left(3 - \frac{5}{3}\right)\theta_1 - \frac{1}{6}$$

$$\Rightarrow \frac{7}{6} = \cancel{2}\,\frac{4}{3}\theta_1$$

$$\Rightarrow \theta_1 = \frac{7}{8} = 0.875$$

$$\theta_2 = \frac{5}{13}\left(\frac{7}{8} + \frac{1}{10}\right) = 0.375$$

$$\theta_3 = 0.25$$

$$\theta_4 = 0.625$$

* do again

ξ	Anal.	Num
0		1
0.25		0.382353
0.5		0.147060
0.75		0.058823
1		0.029412

Not much improvement
(Mesh Refinement to better)

Gravity Pendulum

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

$\beta = 10$

$M = 6$

$\theta(t=0) = 0.7$

$\therefore k = \frac{1}{6}$

$\theta(t=1) = 0.5$

For M equal intervals, using central diff. method.
[each step has non-linear eqn, so in each step, we have to use Newton-Raphson method]

for $m_0 = m$,

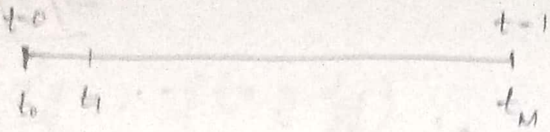
$$\frac{\theta_{m+1} - 2\theta_m + \theta_{m-1}}{k^2} + \beta \sin\theta_m = 0 \qquad k = \frac{1}{M}$$

$$\Rightarrow \theta_{m+1} - 2\theta_m + \theta_{m-1} + \beta k^2 \sin\theta_m = 0$$

We write $f(\theta_m) = \theta_{m+1} - 2\theta_m + \theta_{m-1} + \beta k^2 \sin\theta_m$

We will go from $m = 1$ to $m = M-1$.

$$\cdots - 2z_7 + z_8 - k^2 \gamma z_7 \exp\left(\frac{-\alpha}{z_7}\right) = f_7$$



NR Method

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

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

Here $x = \theta$, $x_1 = \theta_1, \ldots$

m=1

$$\theta_2 - 2\theta_1 + \theta_0 + \beta k^2 \sin\theta_1 = f_1$$

$$\Rightarrow \theta_2 - 2\theta_1 + 0.7 + \beta k^2 \sin\theta_1 = f_1$$

$$\cancel{\frac{\partial f_1}{\partial \theta_1} = -2}, \quad \cancel{\frac{\partial f_1}{\partial \theta_2} = 1}$$

$$\frac{\partial f_1}{\partial \theta_1} = -2 + k^2 \beta \cos\theta_1, \quad \frac{\partial f_1}{\partial \theta_2} = 1$$

m=2

$$\theta_3 - 2\theta_2 + \theta_1 + \beta k^2 \sin\theta_2 = f_2$$

$$\frac{\partial f_2}{\partial \theta_1} = 1, \quad \frac{\partial f_2}{\partial \theta_2} = -2 + k^2 \beta \cos\theta_2, \quad \frac{\partial f_2}{\partial \theta_3} = 1$$

m=3

$$\theta_4 - 2\theta_3 + \theta_2 + \beta k^2 \sin\theta_3 = f_3$$

$$\frac{\partial f_3}{\partial \theta_4} = 1, \quad \frac{\partial f_3}{\partial \theta_3} = -2 + k^2 \beta \sin\theta_3$$

$$\frac{\partial f_3}{\partial \theta_1} = 0, \quad \frac{\partial f_3}{\partial \theta_2} = 1$$

27/3/19

Gravity Pendulum

Initial guess => 0.6 for all θ's

Final Answer: $\theta_1 = 1.3455$

$\theta_2 = 1.7203$

$\theta_3 = 1.8204$

$\theta_4 = 1.8513$

$\theta_5 = 1.2054$

Cross Check

— o —

Shooting Methods

Used for 2^{nd} or higher order BVP. In this method,

① We convert the BVP to an IVP. For that we convert the higher order ODE into a set of lower order ODE.

② Boundary conditions are given to us, but we need the Initial Condition. We need to formulate the Initial Condition (guess)

③ Employ IVP solver.

④ Convergence Check. [We need to iteratively find the guess value of initial condition for convergence]

Linear Interpolation   Newton-Raphson/Secant

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

Example

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

BC: $$y(x=a) = \alpha$$
$$y(x=b) = \beta$$

Steps

① Higher order ODE to set of lower order ODE.

$y = y_1 \rightarrow$ Assumption

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

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

②

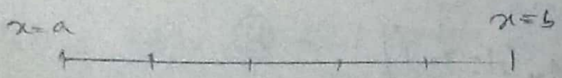
IC: $y_1(x=a) = \alpha$ [from BC 1]

$y_2(x=a) = ?$ [not known]

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

$y_2(x=a) = y_{20}$ (guess)

③



With the guess IVP, we solve, find $y(x=b)$ and check if

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

Explicit Euler (say we use):

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

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(4) $\left| y_{1,m+1} - y_1(x=b) \right| \le tol$??

$\downarrow$

@ $x=b$

Ex-1 (Shooting + RK-4 + Newton-Raphson)

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

$M = 3$, $tol = 10^{-3}$

BCs : $y(0) = 0$

$y(9) = 0$

Soln:

$y = 0$ ... $y = 0$

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

$k = \frac{9}{3} = 3$

Let $y = y_1$

$\therefore \frac{dy_1}{dx} = y_2$ — (i)

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

IC1 : $y_1(0) = 0$ (known)

IC2 : $y_2(0) = 4$ (let)

$y_{1,m+1} = y_{1,m} + k\, y_{2,m}$ — (a)

$y_{2,m+1} = y_{2,m} + k\left[5y_{1,m} + 10x_m(1-x_m)\right]$ — (b)

$y_{1,1} = y_{1,0} + 3 \times y_{2,0} = 0 + 3\times 4 = 12$

$y_{2,1} = y_{2,0} + 3\times\left[5y_{1,0} + 10\underset{0}{x_0}(1-x_0)\right] = 4 + 3\times 5\times 0 = 4$

$y_{1_2} = y_{1_1} + 3 \times y_{2_1} = 12 + 3 \times 4 = 24$

$y_{2_2} = y_{2_1} + 3[5 y_{1_1} + 10 x_1 (1 - x_1)] = 4 + 3[5 \times 12 + 10 \times 3 (1-3)]$

$= 4$

$y_{1_3} = y_{1_2} + 3 y_{2_2} = 24 + 3 \times 4 = 36$ [$\neq 0$ which is the actual value of $y(9)$. So, take another guess].

2nd guess

Let IC2 : $y_2(0) = -2$

$y_{1_1} = y_{1_0} + 3 y_{2_0} = 0 + 3 \times (-2) = -6$

$y_{2_1} = y_{2_0} + 3[5 y_{1_0} + 10 x_0 (1 - x_0)] = -2$

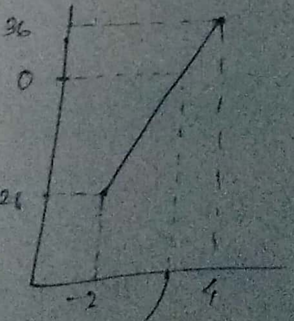
$y_{1_2} = y_{1_1} + 3 y_{2_1} = -6 + 3 \times (-2) = -12$

$y_{2_2} = y_{2_1} + 3[5 y_{1_1} + 10 x_1 (1 - x_1)] = -2 + 3[5 \times (-6) + 10(3)(1-3)]$

$= -272$

$y_{1_3} = y_{1_2} + 3 y_{2_2} = -828$ [$\neq 0$ which is the actual value of $y(9)$.
We took the 2 guesses such that the actual soln $y(9) = 0$ is in b/w the 2 guessed soln.]

Interpolating the Initial Condition 2 :



$y_3^1 \quad y(x=4)$

$y_3^2 \quad y(x=-2)$

$0 - 36 = \left(\frac{36 + 828}{4 + 2}\right)(x - 4)$

$\Rightarrow x = 3.75$

5

$\therefore$ Let IC_2 : $y_2(0) = 3.75$

IC_1 : $y_1(0) = 0$

$\therefore$

$y_{1_1} = y_0 + 3 \times y_{2_0} = 0 + 3 \times 3.75 = 11.25$

$y_{2_1} = y_{2_0} + 3[5y_{1_0} + 10x_0(1-x_0)] = 3.75$

$y_{1_2} = y_{1_1} + 3y_{2_1} = 11.25 + 3 \times 3.75 = 22.5$

$y_{2_2} = y_{2_1} + 3[5y_{1_1} + 10x_1(1-x_1)] = -7.5$

$y_{1_3} = y_{1_2} + 3y_{2_2} = 22.5 + 3 \times (-7.5) = 0$ ✓

Converged.

How to determine the IC by Secant Method?

Given, BC: $y(x=a) = \alpha$

$y(x=b) = \beta$

Guess values: s^0, s^1

IC: $y_1(x=0) = 0 \quad (=\alpha) \quad$ BC1

$y_2(x=0) = s \quad \ldots$ assumed

$s^0 = \dfrac{\beta - \alpha}{b - a}$ [1st guess value]

Choose s^1 arbitrarily.

Secant Method: $s^{i+1} = s^i - \left(\dfrac{s^i - s^{i-1}}{f^i - f^{i-1}}\right) f^i$

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

[Basically the difference b/w predicted and actual values at $x=b$]

[Use this f for secant Method]

5

Shooting Method

28/3/19

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

$y(x=0) = \alpha$

$y(x=1) = \beta$

Step: Transform to IVP

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

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

ICs: $y_1(x=0) = \alpha$ ... BC1

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

Step 2: IVP Solver (RK2, RK4, Euler, etc.)

Step 3: Convergence check

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

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

Step 4: Generate new guess (Secant Method)

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

$$s^{i+1} = s^i - \frac{s^i - s^{i-1}}{g(s^i) - g(s^{i-1})} g(s^i) \quad \text{--- Secant Method}$$

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

$$\Rightarrow \cancel{s^{i+1} = s^i - \frac{s^i - s^{i-1}}{y(s^i) - y(s}}$$

$$\Rightarrow s^{i+1} = s^i - \frac{s^i - s^{i-1}}{y(1,s^i) - y(1,s^{i-1})}\left[y(1,s^i) - \beta\right]$$

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

$$s^1 = y_2(0) \quad \text{(assume arbitrarily)}$$

For N-R Method

Here, we need only one s value $\left[s^0 = \frac{\beta - \alpha}{1-0}\right]$

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

$$= s^i - \frac{g(s^i)}{\frac{dy_1}{ds}(1,s^i)}$$

But how to get $\frac{dy_1}{ds}(1,s^i)$? [difficult]

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

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

Now,

$$\frac{dy_3}{dx} = \frac{d}{dx}\left(\frac{\partial y_1}{\partial s}\right) = \frac{\partial}{\partial s}\left(\frac{dy_1}{dx}\right) = \frac{dy_2}{ds} = y_4$$

$$\Rightarrow \frac{dy_3}{dx} = y_4 \quad \text{—(3)}$$

$$\frac{dy_4}{dx} = \frac{d}{dx}\left(\frac{\partial y_2}{\partial s}\right) = \frac{\partial}{\partial s}\left(\frac{dy_2}{dx}\right) = \frac{\partial}{\partial s} f(x, y_1, y_2)$$

$$\Rightarrow \frac{dy_4}{dx} = \frac{\partial}{\partial s} f(x, y_1, y_2)$$

$$= \frac{\partial f}{\partial x} \cdot \overset{0}{\cancel{\frac{\partial x}{\partial s}}} + \frac{\partial f}{\partial y_1} \cdot \frac{\partial y_1}{\partial s} + \frac{\partial f}{\partial y_2} \cdot \frac{\partial y_2}{\partial s}$$

$$= \frac{\partial f}{\partial y_1} \cdot y_3 + \frac{\partial f}{\partial y_2} \cdot y_4 \quad \text{—(4)}$$

The IVP problem becomes [Step 1 : Transform to IVP]

$$\frac{dy_1}{dx} = y_2 \quad \text{—(1)}$$

$$\frac{dy_2}{dx} = f(x, y_1, y_2) \quad \text{—(2)}$$

$$\frac{dy_3}{dx} = y_4 \quad \text{—(3)}$$

$$\frac{dy_4}{dx} = y_3 \cdot \frac{\partial f}{\partial y_1} + y_4 \cdot \frac{\partial f}{\partial y_2} \quad \text{—(4)}$$

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

$y_1(0) = \alpha$ given IC1

$y_2(0) = s$ assumed IC2

$y_1(0, s) = \alpha$

$\therefore \frac{\partial y_1}{\partial s}(0, s) = y_3(0, s) = \frac{\partial \alpha}{\partial s} = 0$

$\therefore y_3(0, s) = 0$ IC3

$y_2(0, s) = s$

$\therefore \frac{\partial y_2}{\partial s}(0, s) = y_4(0, s) = \frac{\partial s}{\partial s} = 1$

$\therefore y_4(0, s) = 1$ IC4

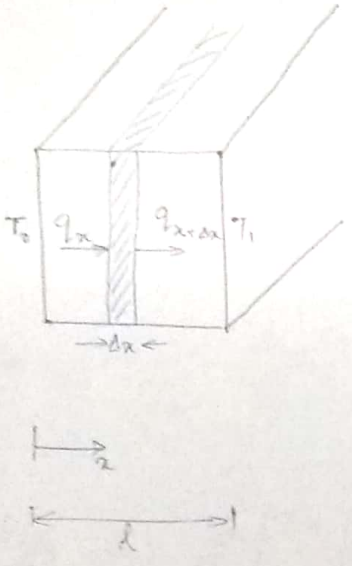
$$\therefore s^{i+1} = s^i - \frac{g(s^i)}{\frac{dy_1}{ds}(1, s^i)}$$

$\frac{dy_1}{ds}(1, s^i) = y_3(1, s^i)$

We need to solve the 4 ODE (IVPs) to get y_3 expⁿ to get $y_3(1, s^i)$. Then we update s^{i+1}

5

Example (Case Study)



Assumptions

- Steady state
- 1D Heat Conduction in x-direction
- No heat generation

$$\therefore \underset{in}{q_x} = \underset{out}{q_{x+\Delta x}}$$

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

$$\Rightarrow \frac{d}{dx}\left(k\frac{dT}{dx}\right) = 0$$

Let k varies with T as:

$$k = k_0 + k_1 (T - T_0)$$

Non-dimensionalizing:

$$\theta = \frac{T - T_0}{T_1 - T_0}$$

$$\xi = \frac{x}{l}$$

$$a = \frac{k_1}{k_0}(T_1 - T_0)$$

$i^2 \propto z_2 \exp\left(-\frac{\alpha}{z_1}\right) \cdot g_7$

$$\frac{d}{dx}\left(k \frac{dT}{dx}\right) = 0$$

$$\Rightarrow \frac{d}{d\xi}\left[\{k_0 + k_1 (T - T_0)\} \frac{dT}{d\xi}\right] = 0$$

$$\Rightarrow \frac{d}{d\xi}\left[\left\{1 + \frac{k_1}{k_0}(T - T_0)\right\} \frac{dT}{d\xi}\right] = 0$$

$$\Rightarrow \frac{d}{d\xi}\left[(1 + a) \frac{dT}{d\xi}\right] = 0$$

$$\Rightarrow \frac{d}{d\xi}\left[(1 + a) \frac{d\theta}{d\xi}\right] = 0$$

$$\Rightarrow (1 + a)\, d^2\theta$$

$$\Rightarrow \frac{d}{d\xi}\left[\left\{1 + \frac{k_1}{k_0}(T - T_0)\right\}(T_1 - T_0) \frac{d\theta}{d\xi}\right] = 0$$

$$\Rightarrow \frac{d}{d\xi}\left[(1 + a\theta) \frac{d\theta}{d\xi}\right] = 0$$

$$\Rightarrow (1 + a\theta) \frac{d^2\theta}{d\xi^2} + a\left(\frac{d\theta}{d\xi}\right)^2 = 0$$

BVP: $(1 + a\theta) \frac{d^2\theta}{d\xi^2} + a\left(\frac{d\theta}{d\xi}\right)^2 = 0$

BC: $\theta(\xi = 0) = 0$

$\theta(\xi = 1) = 1$

Solve by Shooting + explicit Euler + Secant

$M = 10$, $a = 1$

Step 1

$\theta_1 = \theta$

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

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

Step 1

~~BC~~ IC1 : $\theta_1(\xi = 0) = 0$

IC2 : $\theta_2(\xi = 0) = s$

Taking 2 guess values of s

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

$s^1 = 1.2$ (should be $\pm 20\%$ of s^0)

Step 2

$$\frac{\theta_{1_{m+1}} - \theta_{1_m}}{\xi_{m+1} - \xi_m} = \theta_{2_m} \qquad k = \frac{1}{M} = 0.1$$

$$\Rightarrow \theta_{1_{m+1}} = \theta_{1_m} + k\,\theta_{2m} \quad — (3)$$

$$\theta_{2_{m+1}} = \theta_{2m} + k\left[-\frac{\theta_2^2}{1+\theta_1}\right] \quad — (4)$$

Solve till $\theta_{1_{10}}$ and $\theta_{2_{10}}$

Step 3

$$s^2 = s^1 - \frac{s^1 - s^0}{g(s^1) - g(s^0)} \cdot g(s^1) \quad ; \quad g = \theta_1(1, s) - 1$$

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

By shooting + Explicit Euler + N-R

$M = 10, \quad \alpha = 1$

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

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

$$\frac{d\theta_3}{d\xi} = \theta_4 \quad \text{--- (3)}$$

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

$$= \theta_3 \frac{\partial}{\partial \theta_1}\left[\frac{-\theta_2^2}{1+\theta_1}\right] + \theta_4 \frac{\partial}{\partial \theta_2}\left(\frac{-\theta_2^2}{1+\theta_1}\right)$$

$$\frac{d\theta_4}{dx} = \frac{\theta_3 \cdot \theta_2^2}{(1+\theta_1)^2} - \frac{2\theta_2\theta_4}{1+\theta_1} \quad \text{--- (4)}$$

ICs: $\theta_1(0) = 0$

$\theta_2(0) = s^0 = 1$

$\theta_3(0) = 0$

$\theta_4(0) = 1$

$$\boxed{s^{i+1} = s^i - \frac{g(s^i)}{\theta_3(1, s^i)}} \quad \text{N-R}$$

$$s^{i+1} = s^i - \frac{g(s^i)}{\theta_3(1, s^i)} \quad \text{N-R}$$

5

Coupled BVP

29/3/19

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

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

BCs: On y_1 and y_2

x_0	x_1	x_2	$\cdots$	x_M
y_{10}	y_{11}	y_{12}		y_{1M}
y_{20}	y_{21}	y_{22}		y_{2M}

$$\text{Say } Z = \begin{bmatrix} y_{10} \\ y_{11} \\ \vdots \\ y_{1M} \\ \hdashline y_{20} \\ y_{21} \\ \vdots \\ y_{2M} \end{bmatrix} = \begin{bmatrix} z_0 \\ z_1 \\ \vdots \\ z_M \\ \hdashline z_{M+1} \\ z_{M+2} \\ \vdots \\ z_{2M+1} \end{bmatrix}$$

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

Discretizing eqⁿ ① {Central Difference}:

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

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

$$- k^2 \alpha z_2 \exp\left(\frac{-\alpha}{z_1}\right) = g_7$$

So, $g_m = z_{m-1} - 2z_m + z_{m+1} - k^2 f_1(z_m, z_{m+M+1}) = 0$

This g_m will be used for N-R. $\left[z_m^{i+1} = z_m^i - \frac{g(z_m^i)}{g'(z_m^i)} \right]$

Discretizing eq^n 2

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

$$\Rightarrow \frac{z_{m+M+2} - 2z_{m+M+1} + z_{m+M}}{k^2} = f_2(z_m, z_{m+M+1})$$

$$\Rightarrow g_{m+M+1} = z_{m+M} - 2z_{m+M+1} + z_{m+M+2} - k^2 f_2(z_m, z_{m+M+1}) = 0$$

~~Solve the j~~ Get the Jacobian, find the values

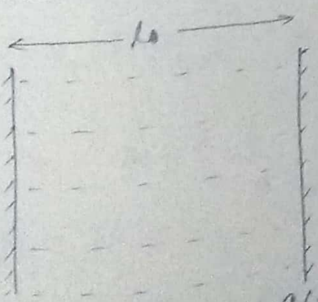
Ex

Reaction - Diffusion System

Assumptions: Steady state, 1D, convection neglected, 1st order rxn

Say, a 1st order rxn occurs

$r = kC$



$C(x=0) = 0$ $\quad C(x=l) = C_0$

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

Model Eq^{n}s:

$$D\frac{d^2C}{dx^2} - k_0 \exp\left(\frac{-E}{RT}\right) C = 0 \quad \ldots (1) \text{ (Mole balance)}$$

$$K\frac{d^2T}{dx^2} + (-\Delta H_r) k_0 \exp\left(\frac{-E}{RT}\right) C = 0 \quad \ldots (2) \text{ (Energy balance)}$$

thermal conductivity

Non - dimensionalizing :

5, $\bar{C} = \frac{C}{C_0}$, $\bar{T} = \frac{T}{T_0}$, $\bar{x} = \frac{x}{l}$, $\alpha = \frac{E}{RT_0}$

Mole Balance :

$$\frac{D\, C_0}{l^2} \frac{d^2 \bar{C}}{d\bar{x}^2} - k_0 \exp\left(-\frac{E}{R T_0 \bar{T}}\right) C_0 \bar{C} = 0$$

$$\Rightarrow \frac{D}{l^2} \frac{d^2 \bar{C}}{d\bar{x}^2} - k_0 \exp\left(-\frac{\alpha}{\bar{T}}\right) \bar{C} = 0 \qquad \cancel{1a}$$

~~Energy Bal~~

$$\Rightarrow \frac{d^2 \bar{C}}{d\bar{x}^2} - \frac{k_0 l^2}{D} \exp\left(-\frac{\alpha}{\bar{T}}\right) \bar{C} = 0$$

Now, $\psi = \sqrt{\frac{k_0 l^2}{D}}$ (Thiele Modulus)

$$\therefore \frac{d^2 \bar{C}}{d\bar{x}^2} - \psi^2 \exp\left(-\frac{\alpha}{\bar{T}}\right) \bar{C} = 0 \quad \text{— (1a)}$$

Energy Balance :

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

$$\Rightarrow \frac{K T_0}{l^2} \frac{d^2 \bar{T}}{d\bar{x}^2} + (-\Delta H_r)\, k_0 \exp\left(-\frac{\alpha}{\bar{T}}\right) C_0 \bar{C} = 0$$

$$\Rightarrow \frac{d^2 \bar{T}}{d\bar{x}^2} \cancel{+} - \frac{k_0 C_0 (\Delta H_r)\, l^2}{K T_0} \exp\left(-\frac{\alpha}{\bar{T}}\right) \bar{C} = 0$$

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

$$\gamma = \frac{k_0 C_0 (\Delta H_r) l^2}{K T_0}$$

$$\therefore \frac{d^2 \bar{T}}{d\bar{x}^2} - \gamma \exp\left(-\frac{\alpha}{\bar{T}}\right) \bar{c} = 0 \quad \text{— (2a)}$$

BCs: $\bar{c}(\bar{x}=0) = 0 \;;\; \bar{c}(\bar{x}=1) = 1$

$\bar{T}(\bar{x}=0) = 1 \;;\; \bar{T}(\bar{x}=1) = 1$

$M = 4$

$$\begin{array}{cccccccc}
 & & \bar{x}=0 & & & & \bar{x}=1 & \\
0 = & & \bar{C}_0 & \bar{C}_1 & \bar{C}_2 & \bar{C}_3 & \bar{C}_4 & = 1 \\
 & & z_0 & z_1 & z_2 & z_3 & z_4 & \\
 & & \bar{T}_0 & \bar{T}_1 & \bar{T}_2 & \bar{T}_3 & \bar{T}_4 & = 1 \\
1 = & & z_5 & z_6 & z_7 & z_8 & z_9 &
\end{array}$$

Discretizing (1a) by Central difference:

$$C_{m-1} - 2C_m + C_{m+1} - k^2 \varphi^2 \exp\left(\frac{-\alpha}{\bar{T}_m}\right) \bar{C}_m = 0 = g_m$$

$$\Rightarrow z_{m-1} - 2z_m + z_{m+1} - k^2 \varphi^2 \exp\left(\frac{-\alpha}{z_{m+M+1}}\right) z_m = 0$$

$$\Rightarrow z_{m-1} - 2z_m + z_{m+1} - k^2 \varphi^2 \exp\left(\frac{-\alpha}{z_{m+5}}\right) z_m = 0 = g_m \quad \text{— (3)}$$

Consider $m = 1, 2, 3$.

$\underline{m=1}$: $\cancel{z_0}^{\,0} - 2z_1 + z_2 - k^2 \varphi^2 \exp\left(-\frac{\alpha}{z_6}\right) z_1 = g_1$

$$\frac{\partial g_1}{\partial z_1} = -2 - k^2 \varphi^2 \exp\left(\frac{-\alpha}{z_6}\right) = g_{11} \;;\; \frac{\partial g_1}{\partial z_2} = 1 = \frac{\partial g}{\partial} = g_{12} ;$$

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

$g_{row,\,column}$ → elements of Jacobian for N-R

5

$m=2$: $z_1 - 2z_2 + z_3 - k^2\varphi^2 z_2 \exp\left(-\frac{\alpha}{z_7}\right) = g_2 \ (=0)$ — (4)

$\frac{\partial g_2}{\partial z_1} = 1 = g_{21}$; $\frac{\partial g_2}{\partial z_2} = -2 - k^2\varphi^2 \exp\left(-\frac{\alpha}{z_7}\right) = g_{22}$

$\frac{\partial g_2}{\partial z_3} = 1 = g_{23}$; $\frac{\partial g_2}{\partial z_7} = -k^2\varphi^2 z_2 \frac{\alpha}{z_7^2} \exp\left(-\frac{\alpha}{z_7}\right) = g_{27}$

$m=3$: $z_2 - 2z_3 + \underset{1}{\cancel{z_4}} - k^2\varphi^2 z_3 \exp\left(-\frac{\alpha}{z_8}\right) = g_3 \ (=0)$ — (5)

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

$\frac{\partial g_3}{\partial z_8} = -k^2\varphi^2 z_3 \frac{\alpha}{z_8^2} \exp\left(-\frac{\alpha}{z_8}\right) = g_{38}$

Discretizing (2a) by Central Difference

$\bar{T}_{m-1} - 2\bar{T}_m + \bar{T}_{m+1} - k^2 \gamma \bar{C}_m \exp\left(-\frac{\alpha}{\bar{T}_m}\right) = 0$

$\Rightarrow z_{m-1+5} - 2z_{m+5} - z_{m+1+5} - k^2\gamma z_m \exp\left(-\frac{\alpha}{z_{m+5}}\right) = 0$

$\Rightarrow z_{m+4} - 2z_{m+5} - z_{m+6} - k^2\gamma z_m \exp\left(-\frac{\alpha}{z_{m+5}}\right) = 0 = g_{m+5}$

Consider $m = 1, 2, 3$.

$m=1$: $\underset{1}{\cancel{z_5}} - 2z_6 + z_7 - k^2\gamma z_1 \exp\left(-\frac{\alpha}{z_6}\right) = g_6$

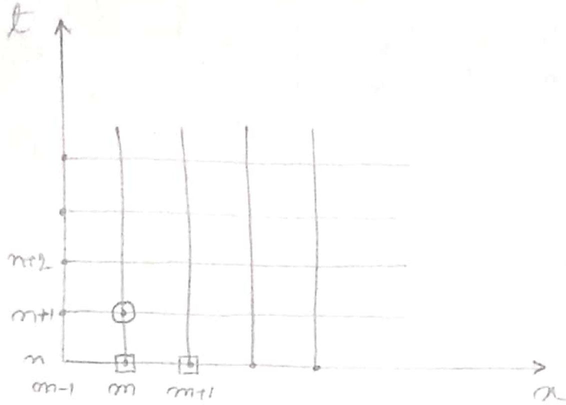
$\frac{\partial g_6}{\partial z_1} = -k^2\gamma \exp\left(-\frac{\alpha}{z_6}\right) = g_{61}$; $\frac{\partial g_6}{\partial z_6} = -2 - k^2\gamma z_1 \frac{\alpha}{z_6^2} \exp\left(-\frac{\alpha}{z_6}\right) = g_{66}$

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

$$\left(\frac{u_m^{n+1} - u_m^n}{h}\right) + a\left(\frac{u_{m+1}^n - u_m^n}{k}\right) = 0 \quad + O(k,h)$$

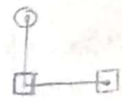
↳ 1st order accurate

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



⊙ = unknown

⊡ = ~~unknown~~ known



Computational Molecule

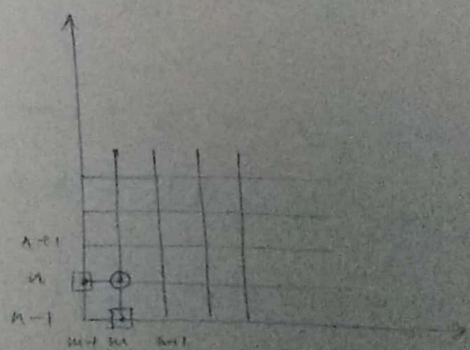
Backward in time & Space (BTBS)

$$\left(\frac{u_m^n - u_m^{n-1}}{h}\right) + a\left(\frac{u_m^n - u_{m-1}^n}{k}\right) = 0 \quad + O(h,k)$$

(first order accurate)

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

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

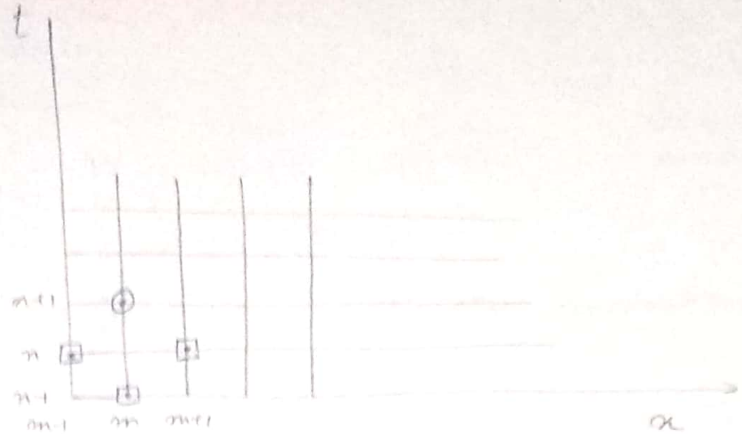


Central in time & space (CTCS)

$$\frac{u_m^{n+1} - u_m^{n-1}}{2h} + a\frac{(u_{m+1}^n - u_{m-1}^n)}{2k} = 0 \quad + O(k^2, h^2)$$

↳ 2nd order accurate

$$\Rightarrow u_m^{n+1} = \frac{h}{k} u_m^{n-1} + \frac{ah}{k}\left(u_{m-1}^n - a u_{m+1}^n\right)$$



For finding $u^n_m, u^n_{m+1}, \ldots$, we need to use either FTFS or BTBS, and from n+1, use CTCS.

Example - 2: Non-linear IBVP

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

BCs: $u(0,t) = t$, $u(1,t) = 1+t$

IC: $u(x,0) = x$, $0 \le x \le 1$

$M = 10$, $h = 0.0001$

Find $u(t=0.25, x)$, $u(t=5, x)$, $u(t=10, x)$

Sol^n: CTCS

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

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

$$\Rightarrow u_{m,n+1} = 2h\cdot u_{m,n-1} + \frac{h}{2k^2}\Big[\left(u_{m+1,n}^2 - 2u_{m+1,n}\cdot u_{m-1,n} + u_{m-1,n}^2\right) + \left(4u_{m,n}\cdot u_{m+1,n} - 8u_{m,n}^2 + 4u_{m,n}u_{m-1,n}\right)\Big]$$

FTFS

Method of lines

We ~~at~~ earlier learnt FTFS, BTBS, and CTCS
1st order accurate, 1st order accurate, 2nd order accurate

We can also use FTCS, CTBS, etc.

In method of lines, we use the other combinations. It is not really a separate line.

Computational Steps:

① Discretize the spatial domain (only)

$x_0 \; x_1 \; - - - - - - \; x_M$

(M+1) nodes.

② Convert the PDE into a set of ODEs (wrt t)

③ Integrate the set of ODEs using the specified BCs and IC.

Ex-1 : One way wave eqn.

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

$\boxed{CS}$

Step 1 & 2 $\quad \frac{du_m}{dt} = -a \frac{(u_{m+1} - u_{m-1})}{2k} \quad m = 1, 2, \dots, (M-1)$

Step 3 Integrate, i.e. use techniques like Euler, RK4 etc. on time.

Let's consider a chemical process

Ex:- Unsteady state 1D Heat conduction

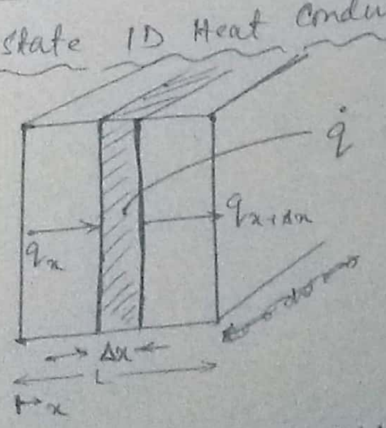
M = 4

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

$T(1, t) = 1$

$T(x, 0) = 2$

$\alpha = 0.00138 \, m^2/min$



q = heat transfer rate

$\dot{q}$ = rate of heat generation per unit volume

Total length = L = 1 m

A = Heat transfer area

$$q_x A_x - q_{x+\Delta x} A_{x+\Delta x} + \dot{q} A \Delta x = \frac{\partial}{\partial t}(\rho A \Delta x \, C_p T)$$

$$\Rightarrow -\frac{\partial q}{\partial x} + \dot{q} = \rho C_p \frac{\partial T}{\partial t}$$

$m=2:\ q_1 - 2q_2 + q_3 - k^2\psi^2 q \exp(-\alpha)$

1D conduction $k\dfrac{\partial^2 T}{\partial x^2} + \dot{q} = \rho C_p \dfrac{\partial T}{\partial t}$

Neglecting $\dot{q}\ (\approx 0)$

$$\Rightarrow \frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

$$\Rightarrow \frac{\partial T_m}{\partial t} = \alpha\frac{(T_{m+1} - 2T_m + T_{m-1})}{k^2} \Rightarrow \frac{dT_m}{dt} = \alpha\frac{(T_{m+1} - 2T_m + T_{m-1})}{k^2}$$

$$\Rightarrow \cancel{\frac{dT_m}{T_{m+1} - 2T_m + T_{m-1}} = \alpha\frac{dt}{k^2}}$$ Applying Euler method (forward Diff.)

$k = 0.25\ (1/M = \frac{1}{4})$

$h = 0.025$

$$T_{m,n+1} = T_{m,n} + h\frac{dT_m}{dt}$$

[FTCS]

$$\Rightarrow T_{m,n+1} = T_{m,n} + h\cdot\alpha\frac{(T_{m+1,n} - 2T_{m,n} + T_{m-1,n})}{k^2}$$

For $m=1$

$$T_{1,n+1} = T_{1,n} + h\cdot\alpha\frac{(T_{2,n} - 2T_{1,n} + T_{0,n})}{k^2}$$

$$\Rightarrow T_{1,n+1} = T_{1,n} + h\alpha\frac{(T_{2,n} - 2T_{1,n} + 0)}{k^2}$$

For $m=2$

$$\Rightarrow T_{2,n+1} = T_{2,n} + h\alpha\frac{(T_{3,n} - 2T_{2,n} + T_{1,n})}{k^2}$$

For $m=3$

$$T_{3,n+1} = T_{3,n} + h\alpha\frac{(T_{4,n} - 2T_{3,n} + T_{2,n})}{k^2}$$

$$\Rightarrow T_{3,n+1} = T_{3,n} + h\alpha\frac{(1 - 2T_{3,n} + T_{2,n})}{k^2}$$

For every n, we need to solve 3 simultaneous eq^{n}s

$\Rightarrow$ Write Code

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