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CH3050 PROCESS DYNAMICS & CONTROL ASSIGNMENT - 2

① a) Let ρ be density of reactor contents, F_i be the flow rate in, C_A be the concentration of A in reactor, C_{Ai} be concentration of A at the inlet, V be volume of reactor, T_i be temperature at inlet and T be temperature of reactor.

Also, for convenience, let $k = \alpha e^{-\beta/T}$ $\alpha = 2.4 \times 10^{15}$, $\beta = -2 \times 10^{4}$

Assumptions

① Reactor is uniformly mixed ensuring same T and C_A everywhere

② $\Delta H_{reaction}$ is constant over the prevailing temperature conditions

③ physical properties such as ρ, C_p are also constant

④ Incompressible flow with no hold-up/accumulation ($F_{in} = F_{out} = F_i$)

Mass balance of A :

$$\frac{V dC_A}{dt} = F_i (C_{Ai} - C_A) - kC_A$$

$$\Rightarrow \frac{dC_A}{dt} = -\left(\frac{F_i}{V} + \alpha e^{-\beta/T}\right) C_A + \frac{F_i C_{Ai}}{V} \quad ①$$

Energy balance around the reactor

$$\rho V c_p \frac{\partial T}{\partial t} = \rho F_i c_p (T_i - T) + \left((-\Delta H_R) k C_A\right) V$$

$$\Rightarrow \frac{\partial T}{\partial t} = \frac{F_i}{V} T_i - \frac{F_i}{V} T + \frac{(-\Delta H_R) \alpha e^{-\beta/T}}{\rho c_p} \quad \text{—— ②}$$

c) Hand calculations (linearisation & finding transfer function)

Let $\frac{dC_A}{dt} = f(C_A, T, C_{Ai})$

$f(C_A, T, C_{Ai}) \approx f \Big|_{\substack{\text{steady-state} \\ C_{A,SS},\, T_{SS},\, C_{Ai,SS}}}$ (recognise that $x = \begin{bmatrix} C_A \\ T \end{bmatrix}$; $u = C_{Ai}$)

$$+ \frac{\partial f}{\partial C_A}(C_A - C_{ASS}) + \frac{\partial f}{\partial T}(T - T_{SS}) + \frac{\partial f}{\partial C_{Ai}}(C_{Ai} - C_{AiSS})$$

At steady state $\frac{dC_A}{dt} = 0 \Rightarrow f = 0$

Also, denote deviation variables with a $\sim$ for convenience.

$$\Rightarrow \frac{d\tilde{C}_A}{dt} = -\left(\frac{F_i}{V} + \alpha e^{-\beta/T_{SS}}\right)\tilde{C}_A + \left(\frac{-\alpha\beta e^{-\beta/T_{SS}} C_{ASS}}{T_{SS}^2}\right)\tilde{T}$$

$$+ \frac{F_i}{V}\tilde{C}_{Ai} \quad \text{—— ③}$$

Doing a similar Taylor expansion for $\frac{dT}{dt}$ around steady state,

$$\frac{d\tilde{T}}{dt} = -\left(\frac{\Delta H_R}{\rho C_p}\alpha e^{-\beta/T_{ss}}\right)\tilde{C}_A + \left[-\frac{F_I}{V} - \frac{\Delta H_R \alpha \beta C_{ss}}{\rho C_p T_{ss}} e^{-\beta/T_{ss}}\right]\tilde{T} \quad (4)$$

C_{ss} and T_{ss} are found using fsolve in MATLAB.

$C_{ss} = 0.0193$ mol/ft^3 $T_{ss} = 558.564\,°R$ - $98.89\,°F$

Notice that coefficients are just constant values, so

let
$$\frac{d\tilde{C}_A}{dt} = a_{11}\tilde{C}_A + a_{12}\tilde{T} + b_1\tilde{C}_i$$

$$\frac{d\tilde{T}}{dt} = a_{21}\tilde{C} + a_{22}\tilde{T}$$

Take Laplace transform on both sides

$$\Rightarrow \quad sC_A(s) = a_{11}C_A(s) + a_{12}T(s) + b_1C_i(s) \quad (5)$$

$$sT(s) = a_{21}C(s) + a_{22}T(s) \quad (6)$$

($\because$ initial conditions are 0, $L\left\{\frac{dC}{dt}\right\} = sC(s)$)

$$\Rightarrow \quad (s - a_{11})C_A(s) - a_{12}T(s) = b_1 C_i(s) \quad (7)$$

and $$C_A(s) = \frac{(s - a_{22})T(s)}{a_{21}} \quad (8)$$

Subst ⑧ in ⑦ to get

$$T(s)\left[\frac{(s-a_{11})(s-a_{22})}{a_{21}} - a_{12}\right] = b_1 C_{Ai}(s)$$

$$\Rightarrow T(s) = \frac{a_{21} b_1 C_{Ai}(s)}{\left((s-a_{11})(s-a_{22}) - a_{12}a_{21}\right)}$$

$$\Rightarrow \frac{T(s)}{C_{Ai}(s)} = \frac{a_{21} b_1}{s^2 - (a_{11}+a_{22})s + a_{11}a_{22} - a_{12}a_{21}} \quad \text{—— ⑨}$$

Subst. back in ⑧,

$$\frac{C_A(s)}{C_{Ai}(s)} = \frac{(s-a_{22})\, b_1}{s^2 - (a_{11}+a_{22})s + a_{11}a_{22} - a_{12}a_{21}} \quad \text{—— ⑩}$$

Substituting the values, ~~we sample~~

$$\frac{T(s)}{C_{Ai}(s)} = \frac{0.1283}{s^2 - 0.6996s + 0.114} \quad \text{and} \quad \frac{C_A(s)}{C_{Ai}(s)} = \frac{0.01667s + 1.19\times10^{-4}}{s^2 + 0.6996s + 0.0114}$$

Both the ~~tf~~ transfer functions match the transfer functions obtained in MATLAB.

Question 1 b) Designing Simulink model & Steady-state

First order equations, f(x,u):

```
-(Fi/V+alpha*exp(-beta/x(2)))*x(1) + Fi/V*u(1)
Fi/V*Ti - Fi/V*x(2) - (delta_Hr)/(pho*Cp)*alpha*exp(-beta/x(2))*x(1)
```

Number of states = 2

Differential Equation Editor (Fcn block syntax)

Name: Reactor

# of inputs: 1

dx/dt=

First order equations, f(x,u):

```
-(Fi/V+alpha*exp(-beta/x(2)))*x(1) + Fi/V*u(1)
Fi/V*Ti - Fi/V*x(2) - (delta_Hr)/(pho*Cp)*alpha*exp(-beta/x(2))*x(1)
```

Number of states = 2

x0

```
CAinit
Tinit
```

Total = 2

y =

Output Equations, f(x,u):

```
x(1)
x(2)
```

Model Workspace

Workspace data

Data source: MATLAB Code

MATLAB Code:

```
Ti = 549.67;
Cp = 0.8;
pho = 52;
delta_Hr = -500*10^3;
V = 1200;
Fi = 20;
alpha = 2.4*10^15;
beta = 2*10^4;
Cp = 1.05506*10^3*0.8; % Converted to kJ/l
CAiss = 0.8;
Tinit = 559;
CAinit = 0.0193;
```

```
>> ss_point

 Operating point for the Model Q1_model.
 (Time-Varying Components Evaluated at time t=0)

States:
----------
(1.) Q1_model/Reactor Model/Integ1
      x: 0.0193
(2.) Q1_model/Reactor Model/Integ2
      x: 559

Inputs:
----------
(1.) Q1_model/FR
      u: 0.8
```

Steady State values obtained using **findop**:

$C_{A,ss}$ = 0.0193 lb/ft^3

T_{SS} = 558.564 Rankine = 98.894 Fahrenheit

Question 1 c) Transfer function form

From c_{Ai} to c_A

```
>> G(1)

ans =

   0.01667 s + 0.0001194
  ------------------------
  s^2 + 0.6996 s + 0.01138

Continuous-time transfer function.
```

From c_{Ai} to T_i

```
>> G(2)

ans =

           0.1283
  ------------------------
  s^2 + 0.6996 s + 0.01138

Continuous-time transfer function.
```

Verified using hand calculations in hand written part

Question 1d): Step response for 10% step change in C_{Ai}

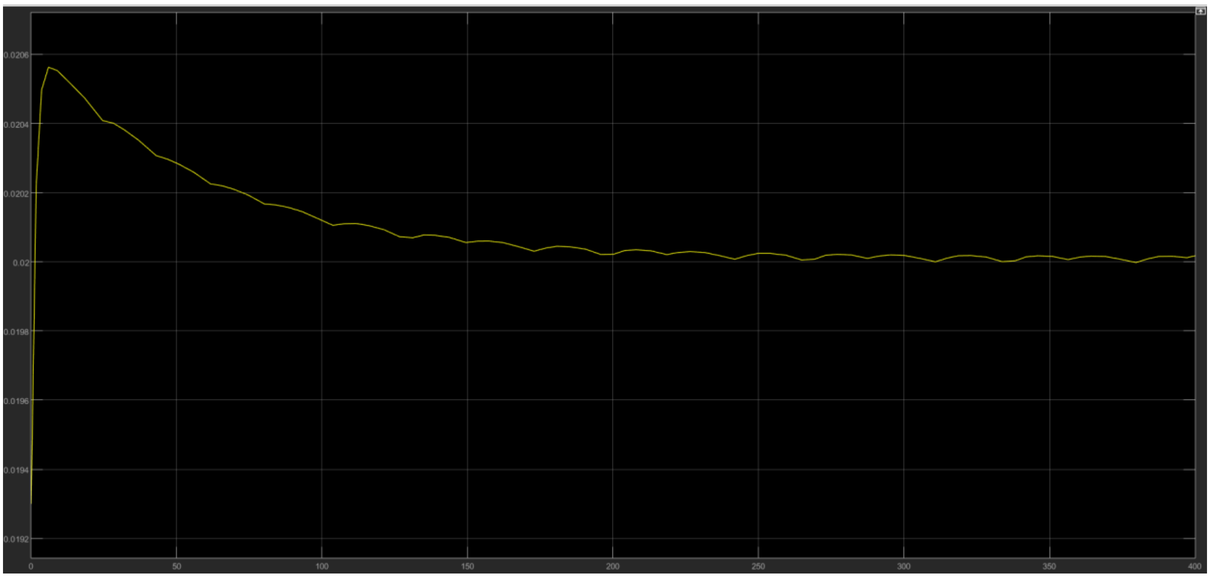


Figure 1: C_A response (non linear model)

$C_{A,ss}$ = 0.0200 (obtained from out.yout)

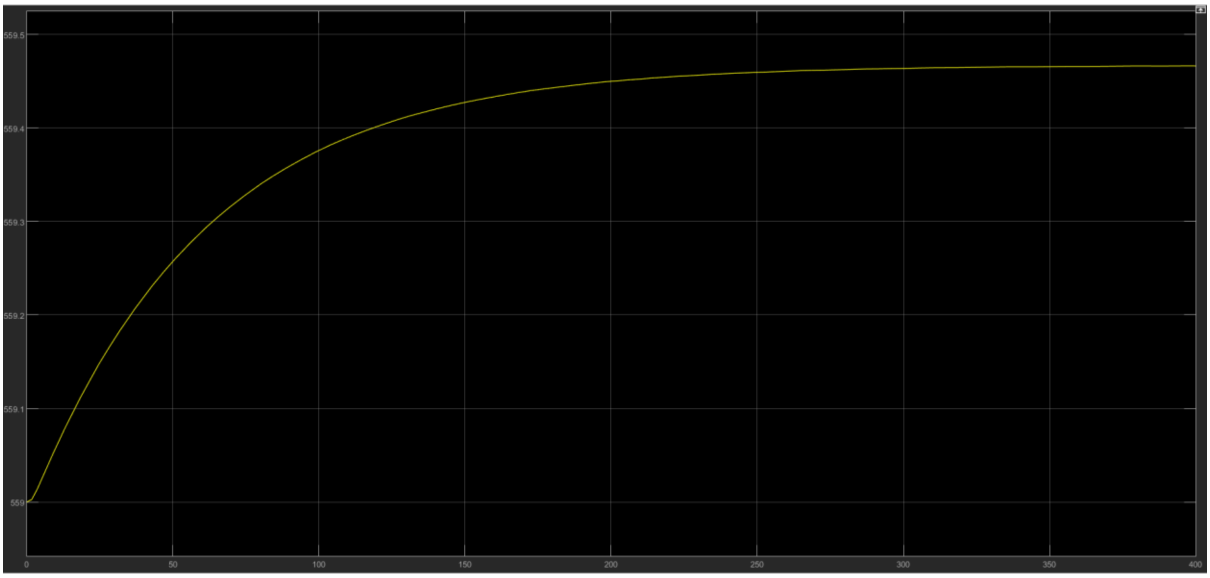


Figure 2: T response (non-linear model)

T_{ss} = 559.4663 Rankine = 99.7963 Fahrenheit

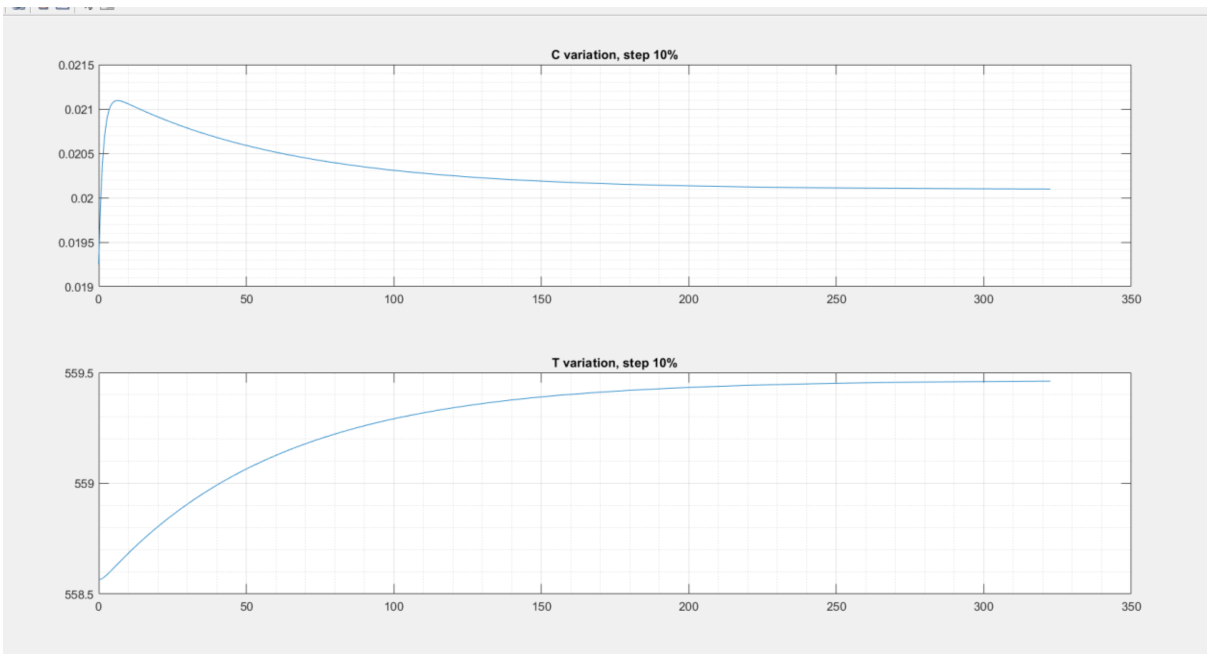


Figure 3: Response from linear models

$C_{A,ss}$ = 0.0201 and **T_{ss} = 559.462 Rankine = 99.792 Fahrenheit**

% error in **$C_{A,ss}$**: 0.5 % and % error in **T_{ss}**: 0.004%. We see that the errors are not huge. So for computational simplicity we can adopt a linear model (provided input conditions aren't altered much)

Question 1 e)

Gain_C = (0.2-0.0193)/0.08 = 2.2588

Gain_T = (559.4663-558.564)/0.08 = 11.278

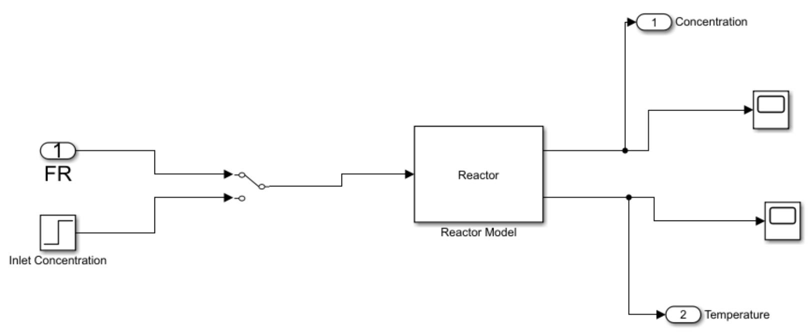
From the gains we can see that for a unit change in input variable, **Temperature** of reactor is affected more than the **concentration of A** in the reactor.

MATLAB Code

```
clear; close all;
%% Part b) Find steady-state and linearise
open_system('Q1_model')
% Read the operating conditions into an object
opc = operspec('Q1_model');
% Operating conditions
opc.Inputs.u = 0.8;
opc.Inputs.Known = 1;
% Constraints
%opc.States(1).Min = 0;opc.States(2).Min = 0;
%opc.States(1).Max = 0.8;
% Find the steady state point
ss_point = findop('Q1_model',opc);
% Linearize
linsys = linearize('Q1_model',ss_point); %Using lin mod: linmod('Q3_model',x_ss,[80 100])
[NUM, DEN] = ss2tf(linsys.A,linsys.B,linsys.C,linsys.D);
```

```
NUM = {NUM(1,:) NUM(2,:)};
G = tf(NUM,DEN);
%% Hand calculations
Css=ss_point.States(1).x;
Tss=ss_point.States(2).x;
Ti = 549.67;
Cp = 0.8;
pho = 52;
delta_Hr = -500*10^3;
V = 1200;
Fi = 20;
alpha = 2.4*10^15;
beta = 2*10^4;
Cp = 1.05506*10^3*0.8; % Converted to kJ/lb
CAiss = 0.8;
Tinit = 559;
CAinit = 0.0193;
A =  zeros(2);
A(1,:) = [-(Fi/V + alpha*exp(-beta/Tss))  -alpha*exp(-beta/Tss)*beta/Tss^2*Css];
A(2,:) = [-delta_Hr/(pho*Cp)*alpha*exp(-beta/Tss) -delta_Hr/(pho*Cp)*alpha*exp(-
beta/Tss)*beta/Tss^2*Css-Fi/V];
B = [Fi/V;0];
C = eye(2);
%% Part d): Computing response
% Since linear system, changes in input and output are proportional
[Y,T,X]=step(linsys);
figure();
subplot(2,1,1);plot(T,Y(:,1)*0.1*0.8+Css); title('C variation, step 10%');
grid on; grid minor;
subplot(2,1,2);plot(T,Y(:,2)*0.1*0.8+Tss); title('T variation, step 10%');
grid on; grid minor;
%% Part e): Comparing gains
Gain_T = 0.4663/0.08;
Gain_C = (0.2-0.0193)/0.08;
```

Simulink model:



(3) a) i) $G(s) = \dfrac{s+1}{(s^3+10s^2+31s+30)} = \dfrac{s+1}{(s+3)(s+2)(s+5)}$

$$\Rightarrow \frac{A_1}{(s+2)} + \frac{A_2}{(s+3)} + \frac{A_3}{(s+5)} = \frac{s+1}{(s+3)(s+2)(s+5)}$$

$$\Rightarrow A_1(s+3)(s+5) + A_2(s+2)(s+5) + A_3(s+3)(s+2) = (s+1)$$

$$s = -2 \Rightarrow A_1 = \frac{-\cancel{4}}{(-2)(-3)} = \cancel{4}\ \frac{1}{3}$$

$$s = -3 \Rightarrow A_2 = \frac{-\cancel{2}}{(-2)(+\cancel{1})} = -\cancel{\tfrac{2}{4}}\ 1$$

$$s = -5 \Rightarrow A_3 = \frac{-4}{(-3)(-2)} = -\frac{2}{3}$$

$$\therefore G(s) = \frac{1}{s+3} - \frac{1}{3(s+2)} - \frac{2}{3(s+5)}$$

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

$X_1(s) = \dfrac{U(s)}{s+3}$; $X_2(s) = \dfrac{U(s)}{s+5}$; $X_3(s) = \dfrac{U(s)}{s+2}$

Inverse LT.

~~$x(s+3)$ & $\dot{x}_1 = U(s)$~~

$\Rightarrow \dot{x}_1 + 3x_1 = u(t)$; $\dot{x}_2 + 5x_2 = u(t)$; $\dot{x}_3 + 2x_3 = u(t)$

$\Rightarrow \dot{x}_1 = -3x_1 + u(t)$; $\dot{x}_2 = -5x_2 + u(t)$; $\dot{x}_3 = u(t) - 2x_3$

$$\therefore \boxed{A = \begin{pmatrix} -3 & 0 & 0 \\ 0 & -5 & 0 \\ 0 & 0 & -2 \end{pmatrix} \; ; \; B = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}}$$

Note ~~that~~ $G(s) = \dfrac{X_1(s)}{U(s)} - \dfrac{2}{3}\dfrac{X_2(s)}{U(s)} - \dfrac{1}{3}\dfrac{X_3(s)}{U(s)}$

$$\Rightarrow Y(s) = X_1(s) - \frac{2}{3} X_2(s) - \frac{1}{3} X_3(s)$$

$$\therefore y(t) = x_1(t) - \frac{2}{3} x_2(t) - \frac{1}{3} x_3(t)$$

$$\boxed{C = \begin{bmatrix} 1 & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix}}$$

ii) $G(s) = \dfrac{Y(s)}{U(s)} = \dfrac{s+1}{(s^3+10s^2+31s+30)}$

$$\Rightarrow (s^3+10s^2+31s+30)\,Y(s) = (s+1)\,U(s)$$

Take inverse Laplace Transform.

$$\Rightarrow \frac{d^3y}{dt^3} + 10\frac{d^2y}{dt^2} + 31\frac{dy}{dt} + 30y = \frac{du}{dt} + u$$

[initial conditions are 0 since tf uses deviation variables]

$$\Rightarrow \frac{d^3y}{dt^3} = -10\frac{d^2y}{dt^2} - 31\frac{dy}{dt} + \frac{du}{dt} + u - 30y$$

Integrate,

$$\Rightarrow \frac{d^2y}{dt^2} = -10\frac{dy}{dt} - 31y + u + \int (u - 30y)\,dt$$

Again integrate wrt time,

$$\Rightarrow \frac{dy}{dt} = -10y + \int\left[(u-31y) + \int(u-30y)\,dt\right]dt$$

Integrate wrt time,

$$\Rightarrow y = \int\left[-10y + \int\left\{u-31y + \left(\int(u-30y)\,dt\right)\right\}dt\right]dt$$

Let $x_1 = \int(u-30y)\,dt$

$x_2 = \int\left(u-31y + \int(u-30y)\,dt\right)dt$

$x_3 = y$

$\Rightarrow \dot{x}_1 = u - 30y = -30x_3 + u.$

$\dot{x}_2 = u - 31y + x_1 = x_1 - 31x_3 + u$

$\dot{x}_3 = -10y + x_2 = x_2 - 10x_3$

$$\therefore \boxed{A = \begin{bmatrix} 0 & 0 & -30 \\ 1 & 0 & -31 \\ 0 & 1 & -10 \end{bmatrix} \quad B = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad C = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}}$$

Notice the eigen values of A in second part is same as eigen values of A in first part ($\because$ same system of β same poles of same eig(A) [-3, -5 and -2])

and also if $x = Tw$ then

$$T^{-1} A_{old} T = A_{new}.$$

We can get this form from eigen value decomposition ($\because V^{-1} A_1 V = A_2$)

So $T = V^{-1}$

$$= \begin{bmatrix} 6.1237 & -18.371 & 55.1135 \\ 1.3123 & -6.562 & 32.8084 \\ -5.626 & 11.353 & -22.206 \end{bmatrix}$$

Eigen vector ie inverse obtained from MATLAB.

Note that MATLAB gives $D = \begin{pmatrix} -2 & & \\ & -3 & \\ & & -5 \end{pmatrix}$

so I had to rearrange the V matrix so that it matches my $A1 = \begin{bmatrix} -3 & 0 & 0 \\ & -5 & 0 \\ 0 & & -2 \\ 0 & 0 & \end{bmatrix}$

~~$A_2 = T A T$~~. $x = Tw$

x are states in SS2

W - states in SS1

3 b) $G_{11}(s) = \dfrac{4s+1}{(s+1)(s+3)}$

$$= -\frac{3}{2}\frac{1}{(s+1)} + \frac{11}{2}\frac{1}{s+3} \quad \text{— } 1$$

$$G_{12}(s) = \frac{10s}{(s+2)(s+3)} = -20\frac{1}{s+2} + 30\frac{1}{(s+3)} \quad \text{— } 2$$

We notice that both the transfer functions have a contribution from $\frac{1}{s+3}$ term.

So we can have the subsystem obeying the dynamics of $\frac{1}{s+3}$. $\left(= \frac{X(s)}{U(s)} \right)$ same for ~~the~~ both cases since we need a minimal realisation (we need minimum no of states to preserve observability & controllability)

So let $\dfrac{X_1(s)}{U(s)} = \dfrac{1}{s+1}$

$$\frac{X_2(s)}{U(s)} = \frac{1}{s+2}$$

$$\frac{X_3(s)}{U(s)} = \frac{1}{s+3}.$$

Taking Inverse L.T.

$\Rightarrow \dot{x}_1 = -x_1 + u$; $\dot{x}_2 = -2x_2 + u$; $\dot{x}_3 = -3x_3 + u$

$$y_1 = -\frac{3}{2}x_1 + \frac{11}{2}x_3 \; ; \; y_2 = -20x_2 + 30x_3$$

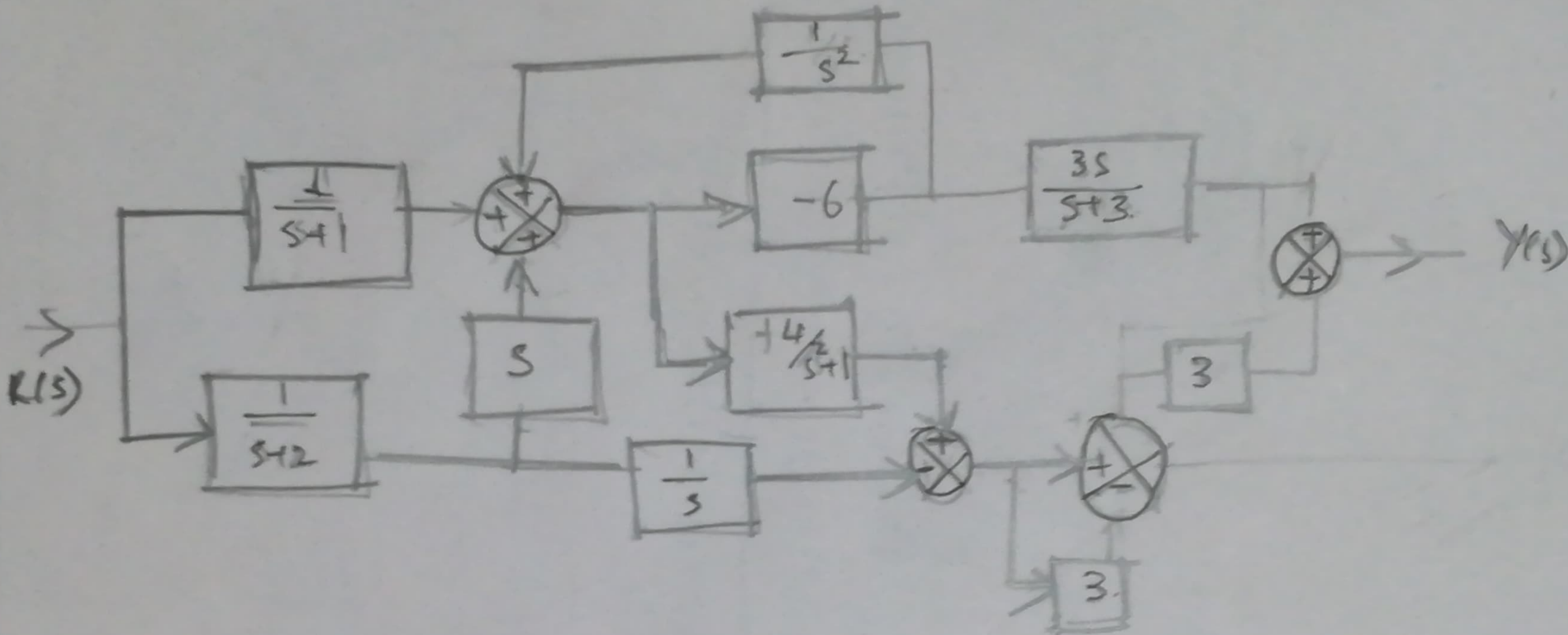
(Obtained by writing eqns ① & ② in terms of $\frac{Y(s)}{U(s)}$ & $\frac{X_k(s)}{U(s)}$ with $U(s)$ cancelling on both sides & then taking inverse Laplace transform).

$$\therefore \boxed{A = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -3 \end{bmatrix} \quad B = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} ; \quad C = \begin{bmatrix} -\frac{3}{2} & 0 & \frac{11}{2} \\ 0 & -20 & 30 \end{bmatrix}}$$

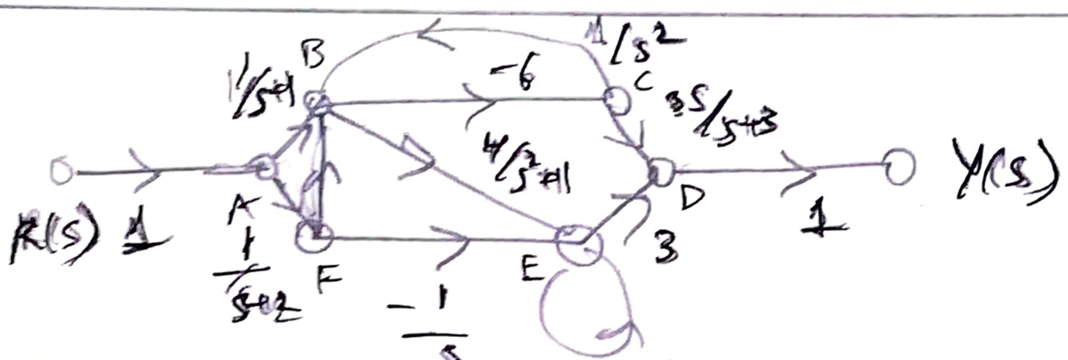
rank of controllability matrix = & rank of observability matrix = 3 = no. of states (evaluated in MATLAB). ∴ system is observable & controllable

⇒ the obtained realisation is indeed the the minimal order realisation

④ i)



(4) ii



Paths	Gain
P_1 : RABCDY	$\dfrac{-18s}{(s+1)(s+3)}$
P_2 : RABEDY	$\dfrac{12}{(s^2+1)(s+1)}$
P_3 : RAFBEDY	$\dfrac{12s}{(s+2)(s^2+1)}$
P_4 : RAFEDY	$\dfrac{-3}{s(s+2)}$
P_5 : RAFBCDY	$\dfrac{-18s}{(s+2)(s+3)}$
L_1 : BCB	$-6/s^2$
L_2 : EE	$-3.$

$$\Delta = 1 - L_1 - L_2 + L_1 L_2 \quad (\because L_1, L_2 \text{ are not touching})$$

$$= 1 + \frac{6}{s^2} + 3 + \frac{18}{s^2} = 4 + \frac{24}{s^2}$$

$\Delta_1 = \Delta\Big|_{L_1=0}$ (only L_1 touches P_1) $= 4$

$\Delta_2 = \Delta\Big|_{L_1=L_2=0}$ (L_1 & L_2 touch P_2) $= \cancel{4}\ 1$

$\Delta_3 = \Delta\Big|_{L_1=L_2=0}$ (L_1 & L_2 touch P_3) $= 1$

$\Delta_4 = \Delta\Big|_{L_2=0}$ (L_2 touches P_4) $= 1+\frac{6}{s^2}$

$\Delta_5 = \Delta\Big|_{L_1=0}$ (L_1 touches P_5) $= 4.$

$\therefore \Delta_1 P_1 = \dfrac{-72s}{(s+1)(s+3)}$ $\qquad \Delta_2 P_2 = \dfrac{12}{(s^2+1)(s+1)}$

$P_3 \Delta_3 = \dfrac{12s}{(s^2+3)(s+2)}$ $\qquad P_4 \Delta_4 = \dfrac{-3\left(1+\frac{6}{s^2}\right)}{s(s+2)}$

$P_5 \Delta_5 = \dfrac{-72s}{(s+2)(s+3)}$

Using the expn for gain

$$\frac{Y(s)}{R(s)} = \frac{\sum_{i=1}^{5} P_i \Delta_i}{\Delta}$$

$$\Rightarrow \frac{Y(s)}{R(s)} = \frac{\frac{-72s}{(s+1)(s+3)} + \frac{12}{(s^2+1)(s+1)} + \frac{12s}{(s^2+1)(s+2)} - \frac{3\left(1+\frac{6}{s^2}\right)}{s(s+2)} - \frac{72s}{(s+2)(s+3)}}{4 + \frac{24}{s^2}}$$

$$= \frac{-72s^{4}(s^2+1)(s+2) + 12s^3(s+2)(s+3) - 3(s^2+1)(s+6)(s+3) + 12s^4(s+3)(s+1) - 72s^4(s^2+1)(s+1)}{4(s^2+6)s(s^2+1)(s+1)(s+2)(s+3)}$$

$$= \frac{-72s^4(s^2+1)(s+2) + 12s^3(s+2)(s+3) - 3(s^2+1)(s+6)(s+3) + 12s^4(s+3)(s+1) - 72s^4(s^2+1)(s+1)}{4(s^2+6)s(s^2+1)(s+1)(s+2)(s+3)}$$