Reactors

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Summary

Determining the optimal reactor conditions and reactor design for the production of specialty chemical C from A and B involves many critical parameters that need to be appropriately accounted for. An analysis based on assumptions was carried out in order to model different reactor designs with the end goal of maximising the profit generated per hour upon operation when using a fixed initial concentration for the limiting reagent A of 1 mol dm^{-3} and a constant reaction solution specific heat capacity of 2500 J kg^{-1} K^{-1}. Computational means were made use of when simulating the reactor designs and numerical methods such as RK4 were employed when solving simultaneous ODES. It was found that adiabatic PFR design allowed for the highest overall maximum achievable profit of 6732.5 \$ h^{-1} when compared to the profit generated by the other reactor designs explored. It was also established that the optimal inlet temperature for the adiabatic PFR design was the lowest at 301.1 K when compared to that estimated for the other reactor designs.

1 Introduction

Optimisation of the production of chemical C that is to be used on the basis of its performance and function is highly desirable [1]. In the production of C involving a reversible reaction [2], a parallel irreversible reaction leading to by-product D also occurs. Out of reagents A and B, A is the crucial reagent that participates in the reaction leading to D [2].

In this investigation different reactor designs were explored with the main objective of identifying the design that would optimise the constrained hourly production of C of 3000 mol h^{-1} by maximising the profits generated [2]. Essential reaction and economic data were available at the onset of the investigation [2].

In the subsequent analysis, the batch reactor design equation 1, the CSTR design equation 2 and PFR design equation 3 were implemented [1,2].

$$r_A = \frac{1}{V_A}\frac{dN_A}{dt} \tag{1}$$

$$V_{CSTR} = \frac{-F_{A0}X_A}{r_A} \tag{2}$$

$$\int_0^{V_{PFR}} dV = \int_0^{X_A} \frac{-F_{A0}dX\prime_A}{r\prime_A} \tag{3}$$

In addition, a uniform density system with ρ at 800 kg m^{-3} for the liquid phase reaction was assumed which was reasonable and also greatly simplified the analysis [1,2].

Energy and molar balances from first principles based on suitable definitions of conversion of A, X and selectivity of C, S [2] were employed throughout the investigation. The reactor systems investigated were also presumed ideal. For instance, steady flow and perfect mixing were implicitly assumed for the CSTR by taking channelling and short-circuiting effects within the reactor as negligible. Moreover, a mean residence time τ was assumed as opposed to also investigating residence time distributions for the CSTR reactor [1]. For the PFR, the plug flow assumption was made which implies perfect radial mixing and negligible axial mixing across the reactor [1].

For each of isothermal batch/PFR, adiabatic batch/PFR, isothermal CSTR and adiabatic CSTR, simulations were carried out computationally by varying critical reaction parameters such as time t, initial concentration of B C_{B0}, temperature T and residence time τ where appropriate [2]. The acceptable operating T ranged from 25 °C to 90 °C and acceptable C_{B0} from 0 to 3 mol dm^{-3} [2]. Additionally, the upper limit constraint on reactor size V was 10 m^3 [2].

The aim was to vary conditions so as to maximise the profit objective function outlined in Appendix 1.A, section 5 [2]. The programming package MATLAB was employed when simulating each reactor design.

There was a particular programming issue with regard to the adiabatic CSTR. The code programmed malfunctioned at the beginning and attempts were made to debug it. Symbolic algebra assignment turned out to be the issue and once this was identified the code was repaired and eventually worked.

In the remainder of this report, the results of the analysis are discussed and, where appropriate, conclusions are made.

2 Results and discussion

2.1 Results

Sample derivations and simulation scripts of the entire investigation with all constraints and decision variables accounted for can be found in Appendix 1.A, section 5.

The following figures and tables serve to act as tools for analysis of the optimal parameter conditions and maximum profit generated for each of the isothermal and adiabatic PFR and CSTR.

Part 1

Table 1: *X*, *S*, volume of reactor required, and max average profit per hour achieved by the use of isothermal batch reaction/PFR at optimum C_{B0}, T_0 and time for reaction.

C_{B0} / mol dm^{-3}	T_0 / K	t / min	V / m^3	X	S	Profit / \$ h^{-1}
1.615	307.1	155.92	10	0.8920	0.8740	6658.2

Figure 1:Plot of selectivity S and conversion X against time for reaction for the optimal choice of *T* / K and C_{B0} / mol dm^{-3} for the isothermal batch reaction/PFR.
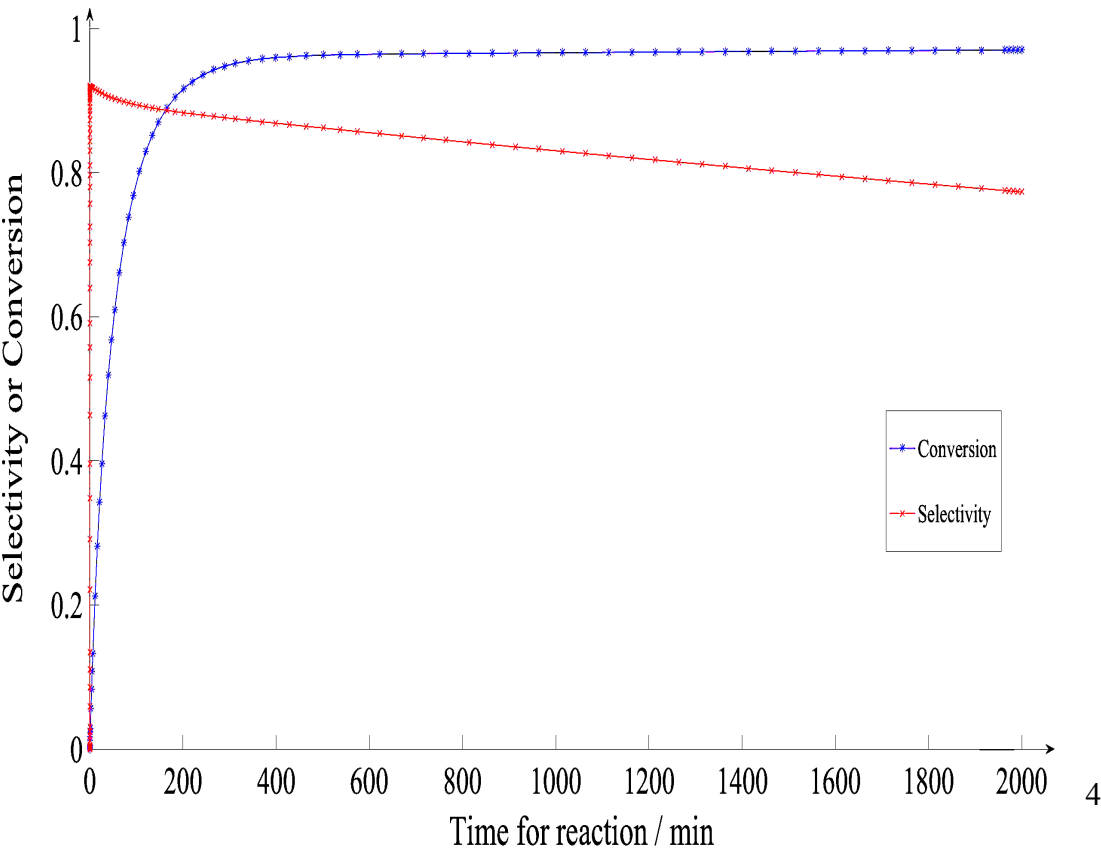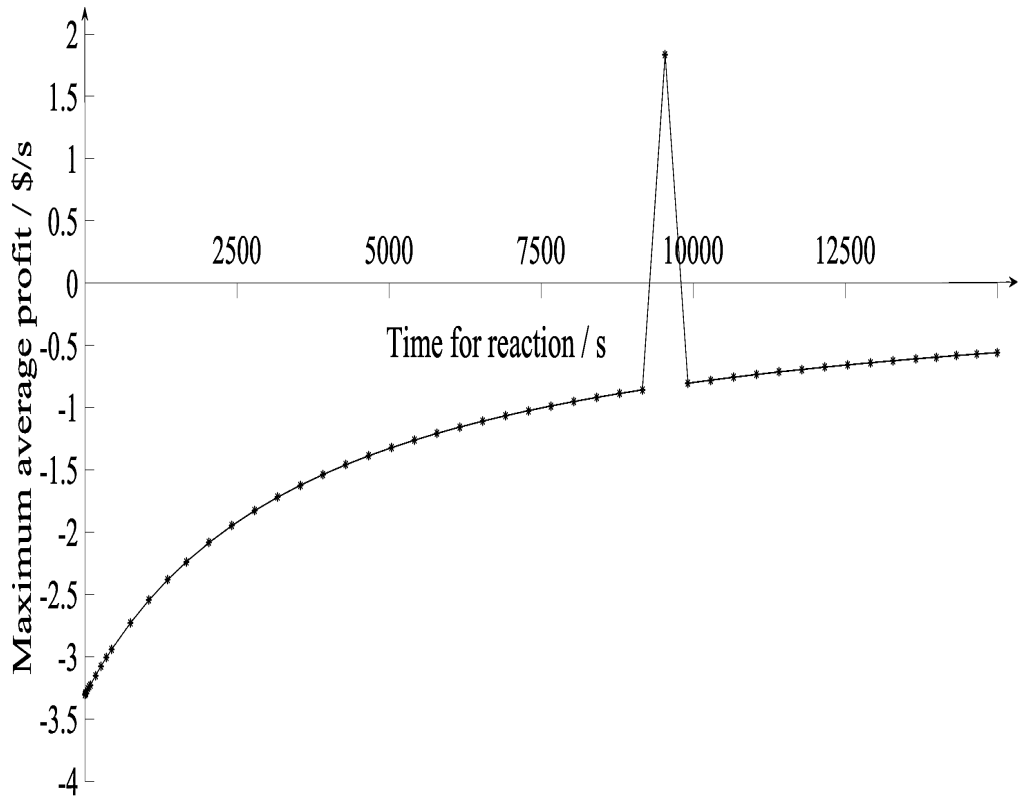
Figure 2: Plot of average maximum profit generated per second against time for reaction, for the optimal choice of *T* / K and C_{B0} / mol dm^{-3} for the isothermal batch reaction/PFR.


4

Part 2

Table 2: X, S, T_{final}, volume of reactor required, and max average profit per hour achieved by the use of adiabatic batch reaction/PFR at optimum C_{B0}, T_0 and time for reaction.

C_{B0} / mol dm^{-3}	T_0 / K	t / min	V / m^3	X	S	T_{final} / K	Profit / $ h^{-1}
1.630	301.1	157.60	10	0.8802	0.8901	309.3	6732.5

Figure 3: 3-D plot of average maximum profit generated per hour on the z-axis against C_{B0} / mol dm^{-3} on the y-axis and T / K on the x-axis for the adiabatic batch reaction/PFR.
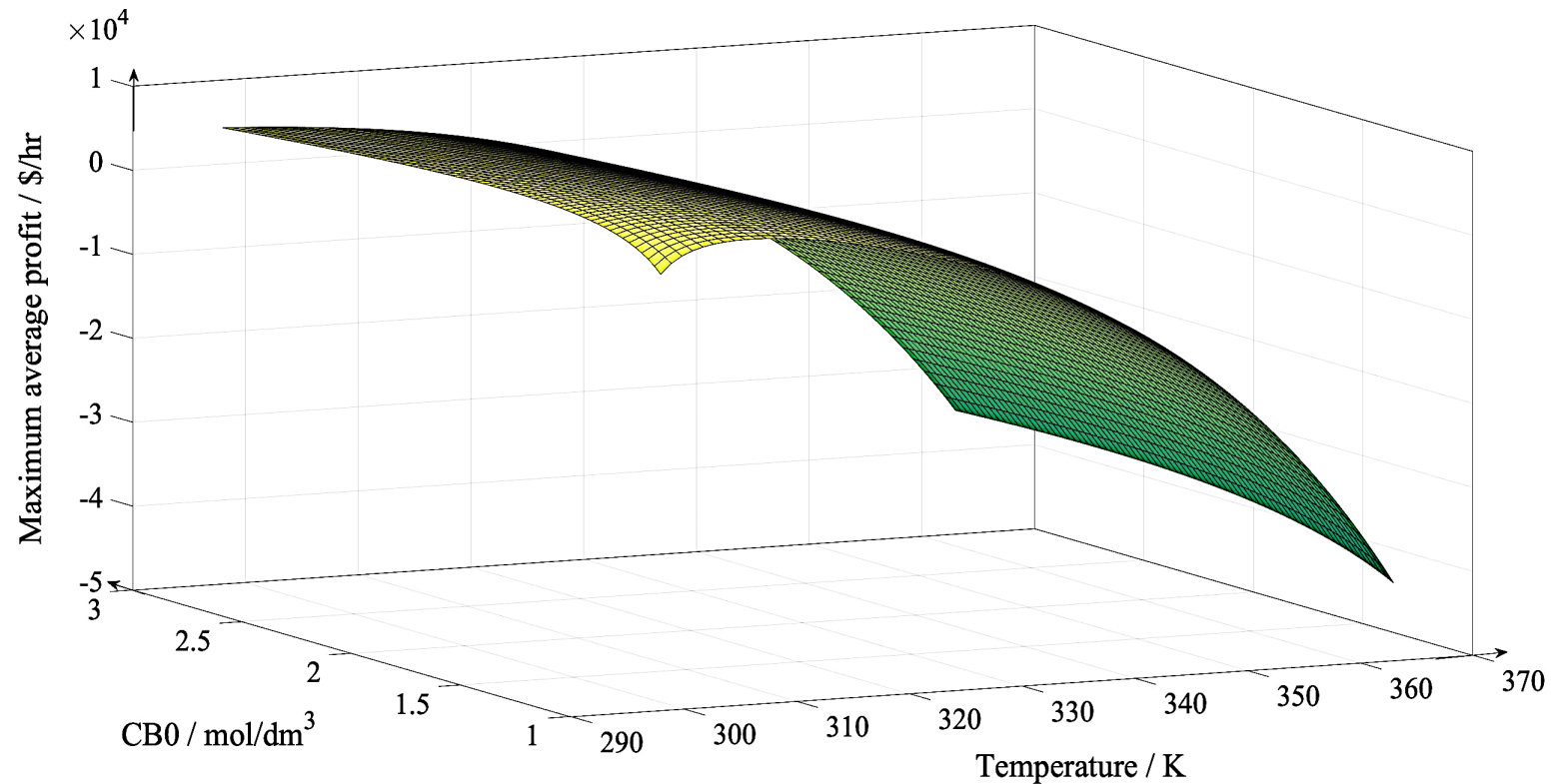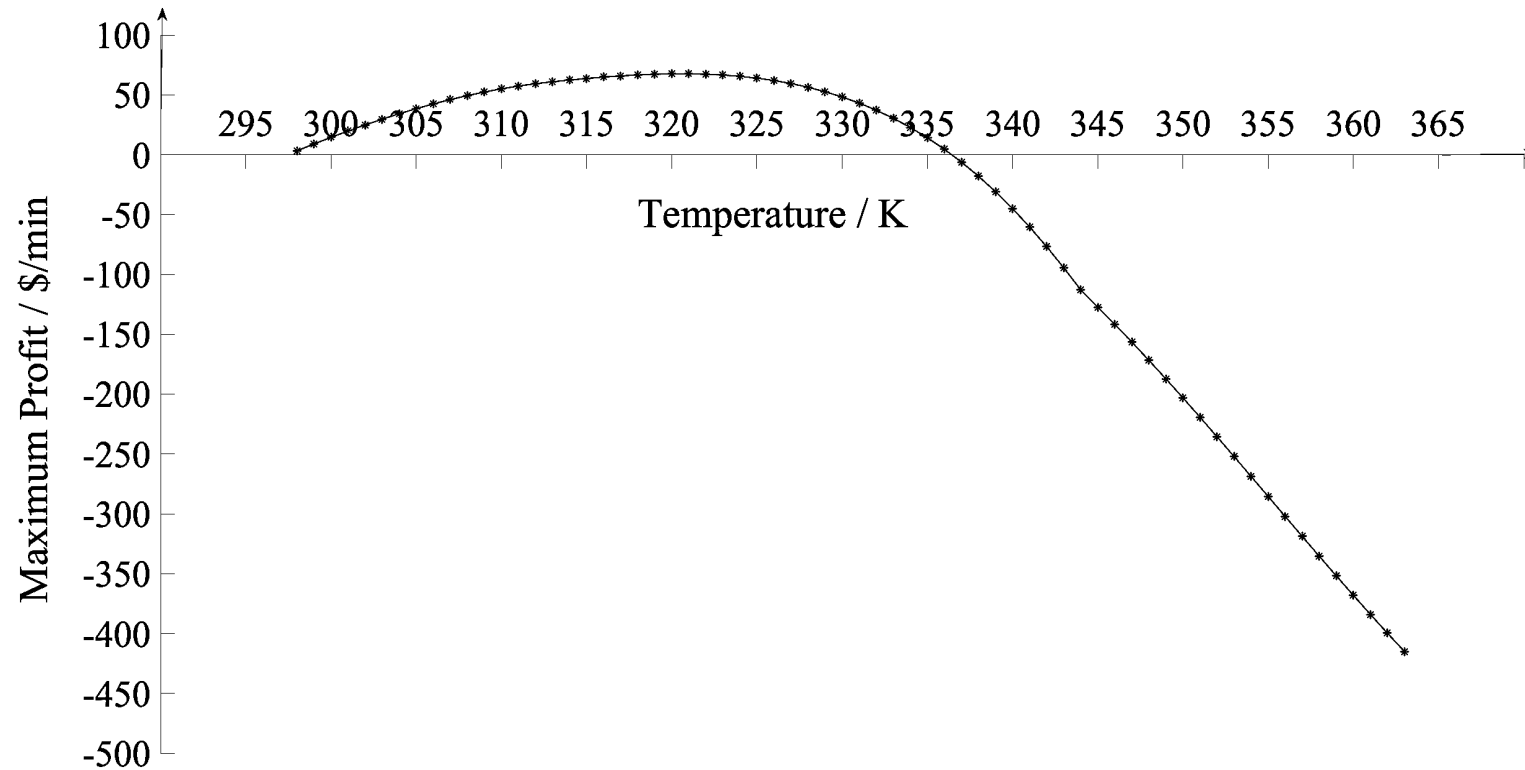
Part 3

Table 3: X, S and max profit per hour achieved by the use of isothermal CSTR at optimum C_{B0}, T_0, mean residence time and volume of reactor.

C_{B0} / mol dm^{-3}	T_0 / K	τ mean / min	V / m^3	X	S	Profit / $ h^{-1}
1.992	321.2	64.97	10	0.7310	0.8510	4049.7

Figure 4: Plot of maximum profit generated per minute against reactor T / K for the optimal choice of mean residence time and C_{B0} / mol dm^{-3} for the isothermal CSTR.

Part 4

Table 4: X, S, T_{out} and max profit per hour achieved by the use of adiabatic CSTR at optimum C_{B0}, T_0, mean residence and volume of reactor.

C_{B0} / mol dm^{-3}	T_0 / K	τ mean / min	V / m^3	X	S	T_{out} / K	Profit / $ h^{-1}
1.993	316.1	98.23	10	0.7499	0.8661	316.2	3821.9

2.2 Discussion

Part 1

Table 1 indicates that the values of S and X achieved for maximum profit of 6658.2 $ h^{-1} match closely at 0.8740 and 0.8920 respectively. They lie near the intersection point of S and X curves depicted in figure 1.

Figure 2 also reveals that at optimally estimated C_{B0} and T tabulated in table 1, there is a net cash flow deficit at any time for reaction other than at roughly 155.92 min.

If an isothermal batch reactor is used there will be an additional 30 min emptying and refill time to account for and since the conditions for the investigation allow τ for batch to be the same as τ for PFR, a PFR would be preferable [1,3,4].

At the desired production rate of C of 3000 mol hr^{-1} on average, with the estimated market for product C lying close to 15 000 000 mol yr^{-1} the PFR would have to be operational for approximately half of each year [2]. Without taking into consideration the costs of the operation, in the scenario that all of C produced at the desired quantity is sold, an income of 150 000 000 USD per annum can be expected if inflation and interest rate fluctuations are ignored [2].

Part 2

Based on tables 1, 2, 3 & 4, use of the adiabatic PFR for which emptying and refill time is not a complication gives rise to the highest maximum profit of 6732.5 \$ h^{-1}. The 3-D plot depicted in figure 3 shows that at any given C_{B0}, at operating T greater than approximately 310 K the maximum average profit in \$ h^{-1} becomes negative. Table 2 reveals that the optimal C_{B0} for the adiabatic PFR is 1.630 mol dm^{-3} which is slightly higher than the 1.615 mol dm^{-3} estimate for the isothermal PFR but lower than the estimates of 1.992 and 1.993 mol dm^{-3} for the isothermal and adiabatic CSTR configurations respectively. Therefore, both the adiabatic and isothermal PFR configurations require the least of reagent B.

In addition, when comparing the estimates of t and τ in tables 1, 2, 3 and 4, the adiabatic PFR has the highest time for reaction at 157.60 min followed closely by the isothermal PFR configuration at 155.92 min. Both, the isothermal and adiabatic CSTR configurations have lower τ in comparison.

Furthermore, the optimal V is the maximum one permitted at 10 m^3 as for all other reactor configurations as well.

Additionally, table 2 reveals that X & S achieved at the optimal conditions for maximising profit in the adiabatic PFR are approximately identical at 0.8802 and 0.8901 respectively as is the case for the isothermal PFR.

Part 3

Tables 1, 2 and 3 reveal that the maximum profit at optimal conditions for the isothermal CSTR of 4049.7 \$ h^{-1} is much less than the maximum profits estimated at optimal conditions for the isothermal and adiabatic PFR configurations.

Moreover, figure 4 shows that for the isothermal CSTR the profit objective function has a maximum that lies at an optimal T_0 of approximately 321.2 K, which is a higher T than the optimal T estimates of both the isothermal and adiabatic PFR configurations.

The CSTR has the advantage that it offers good T control and monitoring as opposed to the PFR [1,3,4]. On the other hand, the PFR offers higher X per unit volume which is also what the data for X in tables 1, 2, 3 & 4 suggest [1]. In order to combine both good T control and higher X per unit volume as well as keep profits generated to a maximum, additional simulations with reactor design configurations incorporating PFR and CSTR in parallel where τ for each branch would have to be the same, could be performed [1].

Further simulations considering the variation in τ across each reactor in residence time distribution diagrams could also be performed so as to establish roughly by how much each reactor design deviates from ideality [1]. Model scales obeying the rules of dynamic and geometric similarity with regard to essential dimensionless groups such as Reynolds number which influence reactor performance could be used to extract vital data for any of the aforementioned additional simulations [1,3].

Part 4

For the adiabatic CSTR configuration, table 4 shows that T_0 and T_{out} are more or less identical at approximately 316 K. Both T_0 and T_{out} for the adiabatic CSTR are lower than T_0 for the isothermal CSTR of 321.2 K but higher than the optimal T estimates made for the isothermal and adiabatic PFR configurations respectively.

The adiabatic CSTR generates the least profit at 3821.9 \$ h^{-1} when compared to the other reactor designs investigated. In addition, as for the isothermal CSTR, both X and S for the adiabatic CSTR as shown in table 4 are less closely matched as opposed to X and S estimates for the isothermal and adiabatic PFR configurations respectively.

PFRs in series could also be considered for design purposes in optimising profits generated. PFRs in series allow for more flexibility in conditions as well as potentially balancing any additional capital cost by significantly reducing operating costs [1,4].

3 Conclusions

The optimum values of fundamental parameters in the investigation for each of the reactor designs investigated with the aim of maximising profits generated were effectively and quantitatively established. It can be concluded that, out of the reactor designs analysed, the adiabatic PFR generates the greatest maximum profits at 6732.5 $ h^{-1}.

In addition, it can be conclusively said that the PFR designs generate maximum profit at lower operating T than the CSTR designs and by also requiring less C_{B0} according to tables 1, 2, 3 and 4.

Despite PFR not offering the best of T control, it is highly recommended that the use of PFRs in series is thoroughly investigated in the future and that more simulations are carried out by also taking into account non-ideality in reactor configurations.

Furthermore, the market for C must be monitored on a regular basis so as to ensure that investment in the appropriate reactor design for maximising potential profits is indeed worthwhile.

4 References

[1] O. Levenspiel, 'Chemical Reaction Engineering', third edition, ISBN 978-0-471-25424-9, 1999 John Wile & Sons. Inc.

[2] Chemical Engineering Tripos Part I, Exercise 3 – Reactors, LT 2019, Reactors, Department of Chemical Engineering and Biotechnology, University of Cambridge, p.1-2 with reaction data and economic data.

[3] L. K. E Achenie, L. T Biegler, In: 'Developing Targets for the Performance Index of a Chemical Reactor Network: Isothermal Systems', Department of chemical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, Ind. Eng. Chem. Res. 1988, 27, 1811-1821.

[4] Chemical Engineering Tripos Part I, Homogeneous Reactors course section 2, Analysis of isothermal 'Ideal' Reactor Systems, Department of Chemical Engineering and Biotechnology, University of Cambridge, pages 1-27, MT 2018.

5 Appendices

Appendix 1.A: Sample derivations and simulation scripts for all types of reactors and conditions explored:

Notations and quantities for sample calculations :
_____

→ Reaction rates :

· $r_A = -u_1 C_A C_B + \dfrac{u_1}{K} C_C - u_2 C_A$

· $r_C = \dfrac{-u_1}{K} C_C + u_1 C_A C_B$

· $r_D = u_2 C_A$

→ Equilibrium and rate constants. :

· $u_1 = 4 \cdot 10^6 \exp\left(\dfrac{-50 \cdot 10^3}{8.3145 \cdot T}\right) / (mol\,dm^{-3})^{-1} min^{-1}$

· $u_2 = 1 \cdot 10^{10} \exp\left(\dfrac{-75 \cdot 10^3}{8.3145 \cdot T}\right) / min^{-1}$

· $K = 2 \cdot 10^{-4} \exp\left(\dfrac{30 \cdot 10^3}{8.3145 \cdot T}\right) / (mol\,dm^{-3})^{-1}$

where $\Delta_r \underline{H}_1 = -30\,kJ\,mol^{-1}$ and $\Delta_r \underline{H}_2 = +40\,kJ\,mol^{-1}$

→ Expressions for C_A, C_B, C_D and C_C based on reactions:

$C_A = C_{A_0}(1-x)$

$C_B = C_{B_0} - x\,s\,C_{A_0}$

$C_C = x\,s\,C_{A_0}$

$C_D = (1-s)\,x\,C_{A_0}$

where $\begin{cases} C_{A_0} = 1\,mol\,dm^{-3} \\ (0 < C_{B_0} \le 3)\,mol\,dm^{-3} \end{cases}$

12

Detailed derivations and Sample calculations.

(3.1) Isothermal batch reaction / Isothermal PFR:

Establishing initial conditions for simultaneous ODEs

- $S = \dfrac{C_c}{C_{A_0} - C_A}$ - $X = \dfrac{C_{A_0} - C_A}{C_{A_0}}$

For $t=0$: $dS = \dfrac{\frac{dC_c}{dt}}{-\frac{dC_A}{dt}}$ $dx = -\dfrac{\frac{dC_A}{^0}}{C_{A_0}} = 0$ @ $t=0$.

@ $t=0$:

$\therefore \quad dS = \dfrac{r_c}{-r_A} = \dfrac{-\frac{u_1}{K}\cancel{C_c}^0 + u_1\cancel{C_A}^{C_{A_0}}\cancel{C_B}^{C_{B_0}}}{-\frac{u_1}{K}\cancel{C_c}^0 + u_1\cancel{C_A}^{C_{A_0}}\cancel{C_B}^{C_{B_0}} + u_2\cancel{C_A}^{C_{A_0}}} = \dfrac{C_{B_0}}{C_{B_0} + \frac{u_2}{u_1}}$

where $\dfrac{u_2}{u_1}$ is temperature dependent.

ODEs :

$\dfrac{dx}{dt} = -\dfrac{1}{C_{A_0}}\dfrac{dC_A}{dt} = -\dfrac{1}{C_{A_0}} \cdot r_A$ since it is a constant density system.

$\therefore \dfrac{dx}{dt} = \dfrac{1}{C_{A_0}}\left[u_1 C_A C_B + u_2 C_A - \dfrac{u_1}{K}C_c\right]$

[ODE(2)]:
$\dfrac{dx}{dt} = u_1\left[1-X\right]\left[C_{B_0} - x\,S\,C_{A_0}\right] + u_2(1-x) - \dfrac{u_1}{K}\cdot S \cdot X.$

$\dfrac{dS}{dt} = \dfrac{1}{(C_{A_0}-C_A)}\dfrac{dC_c}{dt} + C_c\left(C_{A_0}-C_A\right)^{-2}\dfrac{dC_A}{dt}.$

$\therefore \dfrac{dS}{dt} = \dfrac{1}{x C_{A_0}}\dfrac{dC_c}{dt} + \dfrac{S}{x C_{A_0}}\dfrac{dC_A}{dt}.$

$\dfrac{dS}{dt} = \dfrac{1}{x C_{A_0}}\cdot r_c + \dfrac{S}{x C_{A_0}}\cdot r_A$

13

$$\frac{ds}{dt} = \frac{1}{x c_{A_0}} \cdot f_c - \frac{s}{x} \cdot \frac{dx}{dt}$$

ODE(II):

$$\therefore \frac{ds}{dt} = \frac{1}{x}\left[u_1(1-x)(c_{B_0} - x s c_{A_0}) - s(1-x)\left[u_1(c_{B_0} - x s c_{A_0}) + u_2\right] \right]$$

$$+ \frac{u_1}{k} \cdot s[s-1]$$

→ Deriving profit objective function:

Define   Profit = P   ∴   P = Income − costs

$$\therefore \quad P = \left[4.5 c_A + 10 c_c - 1 \cdot c_{B_0} - 5 \cdot c_{A_0}\right] \cdot \frac{V}{T}$$

where   P is in $ hr^{-1},   V = 10000 dm^3

and   T = time of reaction in hrs.

→ Deriving production rate constraint:

Constraint: $\dfrac{c_c \cdot V}{T} = 3000$ mol hr^{-1}

where. $c_c = x s c_{A_0}$ and $c_A = c_{A_0}(1-x)$

∴ • objective function: $\boxed{P = \left[4.5 c_A[1-x] + 10 x s c_{A_0} - c_{B_0} - 5 c_{A_0}\right] \cdot \frac{V}{T}}$

• Constraint: $\boxed{\dfrac{x \cdot s \cdot c_{A_0} \cdot V}{T} = 3000 \text{ mol hr}^{-1}}$

14

MATLAB SCRIPT FOR SOLVING THE ODES IN PART 3.1:

```
Cb0 = 1.6;
Ca0 = 1;
T = 307.2;
k1 = (4*10^6)*exp((-50*10^3)/(8.3145*T));
k2 = (1*10^10)*exp((-75*10^3)/(8.3145*T));
K = (2*10^-4)*exp((30*10^3)/(8.3145*T));
fun =  @(t , d) [ (1 - d(1))*(k1*(Cb0 - d(1)*d(2)*Ca0) + k2) - (k1/K)*d(1)*d(2)  ; (1/d(1))*(k1*(1 - d(1))*(Cb0 -
d(1)*d(2)*Ca0) - d(2)*(1 - d(1))*(k1*(Cb0 - d(1)*d(2)*Ca0) + k2)) + (k1/K)*d(2)*(d(2) - 1) ];
tspan = [0,20000];
d0 = [1*10^-12;0];
[t,d] = ode45(@(t,d) fun(t,d) , tspan , d0);
plot(t,d);
```

MATLAB SCRIPT FOR OPTIMISING OBJECTIVE FUNCTION FOR PART 3.1:

```
Ca0=1;
Ar1 = (4*10^6);
e1 = (50*10^3);
Ar2 = (1*10^10);
e2 = 75*10^3;
R = 8.3144598;
MaximumF = zeros(100,4);
MaximumF2 = zeros(100,4);


T = linspace(306,309,10);
Cb0 = linspace(1.59,1.7,100);
F = linspace (10000,10000,100); %Defining critical parameters and intervals over which they are investigated


for i=1:1 %Temperatures T cycle

    for j= 1:100 %Concentrations Cb0 cycle
    K = (2*10^(-4)) * exp(30*10^3 /(R*T(i)));
    k1= Ar1 * exp(-e1 / (R*T(i)));
```

```matlab
    k2=Ar2 * exp(-e2 / (R*T(i)));


    fun = @(t,d) [(1-d(1))*(k1*(Cb0(j) -d(1)*d(2)*Ca0)+k2)-k1/K*d(1)*d(2) ; ((1-d(2))*((1-d(1))*(k1*(Cb0(j) -
d(1)*d(2)*Ca0)+k2)-k1/K*d(1)*d(2))-k2*(1-d(1)))/d(1)];
    tspan = [0,2000];
    d0 = [10^-12; (Cb0(j)/(Cb0(j) + k2/k1))]; %Defining simultaneous ODES with initial condition

     [t,d] = ode45(@(t,d) fun(t,d) , tspan , d0); %Using RK4 numerical method for solving the ODES
    B=[t,d];
    k = size(B);

    for y = 1:k(1)


        if(round(B(y,2)*B(y,3)*Ca0*F(v)/B(y,1),2) == 3000/60)
            B(y,4) = (Ca0*(10*B(y,2)*B(y,3)-4.5*B(y,2)-0.5)-Cb0(j))*F(v)/B(y,1);
            B(y,5) = Cb0(j); %Constraint and objective function(profit)
    end
    [M,U] = max(B(:,4));
    MaximumF(j,1) = M(1);
    MaximumF(j,2) = T(i);
    MaximumF(j,3) = B(U(1),5);
    MaximumF(j,4) = B(U(1),2);
    MaximumF(j,5) = B(U(1),3);
    end


    [M,U] = max(MaximumF(:,1));
    MaximumF2(i,1) = M(1);
    MaximumF2(i,2) = T(i);
    MaximumF2(i,3) = MaximumF(U(1),3);
    MaximumF2(i,4) = MaximumF(U(1),4);
    MaximumF2(i,5) = MaximumF(U(1),5); %Obtaining ideal parameters in 5 column matrix
    end
```

(3.2) Adiabatic batch reaction / PFR :

Energy balance on adiabatic batch :

- neglect $u.E, P.E$ terms, $\dot{w}_s = 0, \bar{\dot{Q}} = 0$

$$\therefore \frac{d(T \cdot \rho \cdot C_p)}{dt} = (-r_{A_1})(-\Delta_r \underline{H}_1) + G(r_{A_2})(-\Delta_r \underline{H}_2)$$

where $\Delta_r \underline{H}_1 = -30 \text{ uJmol}^{-1}$, $\Delta_r \underline{H}_2 = +40 \text{ uJmol}^{-1}$

$r_{A_1} = -u_1 C_{A_0}(1-x)(C_{B_0} - xs C_{A_0}) + \frac{u_1}{K} C_{A_0} x s$

$r_{A_2} = -u_2 C_{A_0}(1-x)$

$$\therefore \rho \cdot C_p \frac{dT}{dt} = 30 \cdot 10^3 \cdot \left[u_1 C_{A_0}(1-x)(C_{B_0} - xs C_{A_0}) - \frac{u_1}{K} C_{A_0} xs \right]$$
$$- 40 \cdot 10^3 \left[u_2 C_{A_0}(1-x) \right]$$

$$\therefore \frac{dT}{dt} = \frac{10^3}{0.8 \cdot 2500} \cdot 1 \left[30 \left[u_1(1-x)(C_{B_0} - xs C_{A_0}) - \frac{u_1}{K} xs \right] \right.$$
$$\left. - 40 \left[u_2(1-x) \right] \right]$$

$$\frac{dT}{dt} = \ell(x, s) \quad \text{utilised when solving ODEs}$$

for part 3.1 to optimise profit objective function.

MATLAB SCRIPT FOR DEFINING ODES TO BE SOLVED, WITH THE ADDITIONAL EQUATION OF TEMPERATURE DIFFERENTIAL WITH RESPECT TO TIME AS A FUNCTION OF X & S, FOR PART 3.2:

```matlab
function Revenue = BatchPFR(Cb0,T0)
R=8.3145;
e1=50*10^3;
e2=75*10^3;
H1=30*10^3;
Ar1=4*10^6;
Ar2=10^10;
keq=2*10^-4;
k10 = Ar1*exp(-e1/(R*T0));
K0 = keq*exp(H1/(R*T0));
k20 = Ar2*exp(-e2/(R*T0));
S = Cb0/(Cb0+(k20/k10));
H = 0.001;
t = 0;
X = 0.000001;
T = T0;
Ca0 = 1;
Profitability = 0;
f = 30000; %defining initial conditions and appropriate parameters based on initial conditions


listS = zeros( f+1 , 1); listX = zeros( f+1 , 1); listt = zeros( f+1 , 1); listProfit = zeros( f+1 , 1); listT = zeros ( f+1 , 1); %storing values of critical output that is to be calculated

listS(1) = S; listX(1) = X; listt(1) = t; listProfit(1) = Profitability; listT(1) = T; %storing initial estimates for further cycles

    for f = 1:f %number of cycles over which output is to be configured
        Q=5;
        k1 = Ar1*exp(-e1/(R*T));
        K = keq*exp(H1/(R*T));
        k2 = Ar2*exp(-e2/(R*T));

        c1 = k1*(1-X)*(Cb0-Ca0*X*S)-(k1/K)*X*S+k2*(1-X); % ODE with dxdt as f(X,S)
        c2 = (1/X)*(c1-k2*(1-X)-S*c1);                   %ODE with dsdt as f(X,S)
        c3 = ((k1*(1-X)*(Cb0-Ca0*X*S)-(k1/K)*X*S)*(3)-(k2*(1-X))*(4))*Q; %ODE with dTdt as f(X,S)
```

18

```matlab
        X = X + H*c1;
        S = S + H*c2;
        T = T + H*c3;
        t = t + H;
        listS(f+1) = S; listX(f+1) = X; listt(f+1) = t;  listT(f+1) = T; %storing first evaluation
            if -0.0001 < 200*X*S-t < 0.0001;%acceptable error range of 0.1% for constraint
                fmax = f;
            end

    end
S_end = Cb0/(Cb0+(k20/k10));  X_end = 0.00001;  t_end = 0;   T_end = T0;
v = 0.001;

listS_end = zeros(fmax+1,1); listX_end = zeros(fmax+1,1); listt_end = zeros(fmax+1,1); listT_end= zeros(fmax+1,1);

listS_end(1) = S_end; listX_end(1) = X_end; listt_end(1) = t_end; listT_end(1) = T_end; %telling it to store end
estimates of output based on optimising objective function

    for i = 1:fmax-1 %number of refined cycles over which final estimates will be made

        k1 = Ar1*exp(-e1/(R*T_end));
        K = keq*exp(H1/(R*T_end));
        k2 = Ar2*exp(-e2/(R*T_end));

        G1 = k1*(1-X_end)*(Cb0-Ca0*X_end*S_end)-(k1/K)*X_end*S_end+k2*(1-X_end);
        G2 = (1/X_end)*(G1-k2*(1-X_end)-S_end*G1);
        G3 = ((k1*(1-X_end)*(Cb0-Ca0*X_end*S_end)-(k1/K)*X_end*S_end)*(3)-(k2*(1-X_end))*(4))*Q;

        X_end = X_end + v*G1;  S_end = S_end + v*G2; T_end = T_end + v*G3; t_end = t_end + v;

        listS_end(i+1) = S_end;  listX_end(i+1) = X_end;  listt_end(i+1) = t_end; listT_end(i+1) = T_end;
    end

    Ans= Ca0*(-5+4.5*(1-listX_end(fmax))-Cb0+10*listS_end(fmax)*listX_end(fmax)); %profit objective function
    Revenue = Ans*(6*10^5)/(listt_end(fmax)); %listing the maximum average profit per hour
    fmax
    listX_end(fmax)
    listS_end(fmax) %documenting X and S at optimal conditions for maximising profit
end
```

MATLAB SCRIPT FOR OBTAINING MAX AVERAGE PROFIT PER HOUR AND OPTIMAL C_{B0} AND T_0 FOR PART 3.2:

```matlab
T0 = linspace(298,363,50);
Cb0 = linspace(1,3,50); %creating matrices for cb0 and T0 values within accepted range
Ca0 = 1;
Revenueline = zeros(50,50);% Profit matrix with matching dimensions for Cb0 and T0
for k=1:50 %cycles for CB0 matching matrix dimensions
    for v=1:50 %cycles for T0 matching matrix dimensions
        Revenueline(k,v) = BatchPFR(Cb0(k),T0(v));% Calculating Profit at CB0 and T0 values based on function
dependence on S,X and T defined in BatchPFR file as ODES
    end
end
TotRevenue= max(Revenueline); %Maximising profit function for each Cb0 and T0
maxoverall = max(TotRevenue) %Finding maximum profit achieved overall
Bestscenario = find(Revenueline==maxoverall); Cb0Magic= Bestscenario - (T0Magic - 1)*100; T0Magic =
floor(Bestscenario/100) + 1; %Evaluating optimal Cb0 and T0 for maximising profit
Cb0best = Cb0(Cb0Magic) %display Optimal Cb0
T0best = T0(T0Magic) %display optimal T0
```

(3.3) **Isothermal CSTA:**

→ Deriving equations in x and s from molar balances !

• **Molar balance on A:**

$$F_{A_0} + r_A \cdot V = F_A \qquad - Q = \text{constant}$$
$$\text{constant density system.}$$

$$\therefore \quad C_{A_0} + r_A \cdot \frac{V}{Q} = C_A \qquad - \text{where } V/Q = \tau \, [\text{residence time}]$$

$$\therefore \quad r_A \cdot \tau = -C_{A_0} \cdot x$$

$$\tau \cdot \left[-u_1 C_{A_0}(1-x)[C_{B_0} - x s C_{A_0}] + \frac{u_1}{k} C_{A_0} \cdot x \cdot s - u_2 C_{A_0}(1-x) \right]$$

$$= -C_{A_0} \cdot x$$

$$\therefore \boxed{\tau u_1(1-x)(C_{B_0} - x s C_{A_0}) - \frac{\tau u_1}{k} x \cdot s + \tau u_2(1-x) = x} \quad (eq. 1)$$

• **Molar balance on D:**

$$r_D \cdot \frac{V}{Q} = C_D \qquad \text{where } r_D \text{ is rate @ which } D \text{ appears}$$
$$\text{and } C_D \text{ is the concentration of}$$
$$D \text{ as a function of } s \text{ and } x$$

$$\therefore \quad r_D \cdot \tau = (1-s) \cdot x \cdot C_{A_0}$$

$$\therefore \quad u_2 C_{A_0}(1-x) \cdot \tau = (1-s) \cdot x \cdot C_{A_0}$$

$$\therefore \boxed{u_2(1-x) \cdot \tau = (1-s) \cdot x} \quad (eq. 2)$$

• **Re-arranging (eq.1) so that $s = f(x, \tau)$:**

$$s = \frac{\tau u_1(1-x) C_{B_0} + \tau u_2(1-x) - x}{x\left[\tau u_1(1-x) C_{A_0} + \frac{\tau u_1}{k} \right]}$$

21

$$\therefore \quad S = \frac{u_1(1-x)C_{Bo} + u_2(1-x) - \frac{x}{\tau}}{x\left[u_1(1-x)C_{Ao} + \frac{u_1}{k}\right]}$$

- Rearranging (eq. 2) so that $S = f(C_x, \tau)$:

$$S = 1 - \frac{u_2\tau[1-x]}{x}$$

- Equating Rearranged (eq. 1) and (eq. 2):

$$1 - \frac{u_2\tau[1-x]}{x} = \frac{u_1(1-x)C_{Bo} + u_2(1-x) - x/\tau}{x\left[u_1(1-x)C_{Ao} + \frac{u_1}{k}\right]}$$

$$\therefore \left[x - u_2\tau(1-x)\right]\left[u_1(1-x)C_{Ao} + \frac{u_1}{k}\right]$$

$$= u_1[1-x]C_{Bo} + u_2(1-x) - x/\tau$$

$$\therefore \quad x u_1(1-x)C_{Ao} + \frac{x u_1}{k} - u_2\tau u_1 C_{Ao}(1-x)^2$$

$$- \frac{u_2\tau u_1}{k}[1-x] = u_1 C_{Bo} - u_1 C_{Bo}x + u_2 - u_2x - x/\tau$$

- Quadratic in x:

$$\therefore \quad x u_1 C_{Ao} - x^2 u_1 C_{Ao} + \frac{x u_1}{k} - u_2\tau u_1 C_{Ao}[1 - 2x + x^2]$$

$$- \frac{u_2\tau u_1}{k} + \frac{u_2\tau u_1}{k}x - u_1 C_{Bo} + u_1 C_{Bo}x - u_2 + u_2 x$$

$$+ x/\tau = 0.$$

- **Coefficients of quadratic in X:**

- coefficients in x^2: $-u_1 C_{A_0} - u_2 \tau u_1 C_{A_0} = a$.

- coefficients in x: $u_1 C_{A_0} + \dfrac{u_1}{K} + 2 u_2 u_1 \tau C_{A_0} + \dfrac{u_2 \tau u_1}{K}$

  $+ u_1 C_{B_0} + u_2 + \dfrac{1}{\tau} = b$

- Constants: $-u_2 \tau u_1 C_{A_0} - \dfrac{u_2 \tau u_1}{K} - u_1 C_{B_0} - u_2 = c$

- Definitions of a, b and c give:

$$\boxed{ax^2 + bx + c = 0.} \quad \text{eq. for } x$$

→ Solving for $ax^2 + bx + c = 0$
  by defining S as a function of x, τ from eq. 2:

$$\boxed{S = 1 - \dfrac{u_2 \tau [1 - x]}{x}}$$

→ Defining the profit objective function:

$P = $ profit where $P = f(C_x, S, \tau)$

$$\therefore \boxed{P = \left(10 \cdot x \cdot S \cdot C_{A_0} - 0.5 C_{A_0} - 4.5 x \cdot C_{A_0} - C_{B_0}\right) \cdot V/\tau}$$

where $V = 10\,000 \, dm^3$ and $\tau = $ residence time.

Constraint: let $F_c = 3000 \, mol \, hr^{-1} = 50 \, mol \, min^{-1}$

$$\therefore \quad 50 = \dfrac{C_c \cdot V}{\tau} = \dfrac{x \cdot S \cdot C_{A_0} \cdot V}{\tau}$$

$$\therefore \quad \boxed{\dfrac{x \cdot S \cdot C_{A_0} \cdot V}{\tau} - 50 = 0}$$

23

MATLAB SCRIPT FOR OPTIMISING PROFIT FOR ISOTHERMAL CSTR IN PART 3.3:

```matlab
ca0 = 1;
V = 10*10^3; %dm^3 max allowed reactor volume
cb0 = 1.992;%optimum cb0 = 1.992 was obtained by adjusting over a range of cb0 from 1 to 3 and recording the maximum
profit

Temp = linspace(298,363,66);%allowed temperature range for operation

dt = 0.2; %time intervals
t_fin = 100; %timespan limit
n = t_fin / dt;

time = linspace(0,t_fin,n);

profitability = zeros(1,numel(Temp));
    x = zeros(n);
    s = zeros(n);
    xs = zeros(n);
    Constraint = zeros(n);
   Combinations = zeros(2,numel(Temp));

for j=1:numel(Temp) %define temperature vector
    T = Temp(j);

    k1 = 4*10^6*exp(-50000/(8.314*T));
    k2 = 10^10*exp(-75000/(8.314*T));
    K = 2*10^-4*exp(30000/(8.314*T)); %equilibrium and rate constants for T range
    ResidenceTime = zeros(1,100);
    ProfitObjectiveFunction = zeros(1,n);
for i=1:n %define residence time array
    t = time(i); %residence time measured in minutes
    a = -k1*ca0 - k1*k2*ca0*t;
    b = k1*ca0 + k1/K + 2*k1*k2*ca0*t + k1*k2*t/K + k1*cb0 + k2 + 1/t;
    c = -k1*k2*ca0*t - k1*k2*t/K - k1*cb0 - k2; %quadratic coefficients for x

    xi = (-b + sqrt(b^2 - 4*a*c)) / (2*a);
    si = 1 - k2*(1-xi)*t/xi;
```

```
    x(i) = xi;
    s(i) = si;
    xs(i) = xi*si; %x*s for every given timestep
    Constraint(i) = xi*si*ca0*V/t - 50; %constraint equation
    ProfitObjectiveFunction(i) = (10*xi*si*ca0 - 0.5*ca0 - 4.5*xi*ca0 - cb0)*V/t; %objective function
    if Constraint(i) < 1 && Constraint(i) > 0 %allowed error for constraint equation
        ResidenceTime(i) = t;
    end
end
    Combinations(2,j) = max(ResidenceTime); %purpose of combinations(2,j) vector
    Combinations(1,j) = T; %purpose of combinations(1,j) vector
    profitability(j) = max(ProfitObjectiveFunction); %optimising to maximise profit
end
```

MATLAB SCRIPT FOR *X* AND *S* AT OPTIMUM CONDITIONS IN PART 3.3:

```
t = 64.965; %optimum residence time
k1 = 4*10^6*exp(-50000/(8.314*T));
k2 = 10^10*exp(-75000/(8.314*T));
K = 2*10^-4*exp(30000/(8.314*T));
cb0 = 1.992; %optimum cb0 established
ca0 = 1;
T = 321; %optimum temperature
a = -k1*ca0 - k1*k2*ca0*t;
b = k1*ca0 + k1/K + 2*k1*k2*ca0*t + k1*k2*t/K + k1*cb0 + k2 + 1/t;
c = -k1*k2*ca0*t - k1*k2*t/K - k1*cb0 - k2; %quadratic coefficients for x
xi = (-b + sqrt(b^2 - 4*a*c)) / (2*a) %obtaining fractional conversion of A at optimum conditions
si = 1 - k2*(1-xi)*t/xi %obtaining selectivity of C at optimum conditions
```

(3.4) Adiabatic CSTR :

→ Deriving equation for T/K as a function of x, s and T_o :

Energy balance for CSTR at steady state :

$$[IN] + [GEN] = [OUT] + [ACC]^{\nearrow 0} /[s.s.A]$$

$$\therefore \quad V \cdot \left[-r_{A_1}(-\Delta_r \underline{H}_1) - r_{A_2}(-\Delta_r \underline{H}_2)\right] = \rho \phi C_p [T - T_o]$$

$\underbrace{\qquad\qquad}_{}$ constant density and heat capacity system.

where $\rho = 800 \, kg\,m^{-3}$
and $C_p = 2500 \, J\, kg^{-1} k^{-1}$

$$r_{A_1} = -k_1 C_A C_B + \frac{k_1}{K} C_C \qquad \& \qquad r_{A_2} = -k_2 C_D$$

$\therefore$ If $\Delta_r \underline{H}_1 = -30 \, kJ\,mol^{-1}$ $\quad \& \quad \Delta_r \underline{H}_2 = +40 \, kJ\,mol^{-1}$

$$\therefore \quad \frac{V}{\phi} \left[-r_{A_1} \cdot 30\,000 + r_{A_2} \cdot 40\,000\right] = \rho C_p [T - T_o]$$

where $\frac{V}{\phi} = \tau$ [residence time]

$$\therefore \quad \frac{\tau}{\rho C_p} \left[\left(k_1 C_{Ao}(1-x) C_{Bo} - x s C_{Ao}\right) - \frac{k_1}{K} C_{Ao} x s\right) \cdot 30\,000 \right.$$
$$\left. + 40\,000 \left(-k_2 C_{Ao}(1-x)\right)\right] = T - T_o.$$

$\therefore$ If C_{Ao} is in $mol\,dm^{-3}$ $\therefore C_{Ao} = 10^3 \, mol\,m^{-3}$

$$\therefore \quad \frac{\tau \cdot 10^7}{800 \cdot 2500} \cdot \left[\quad 3 \cdot \left[k_1(1-x) C_{Bo} - x s C_{Ao}\right) - \frac{k_1}{K} x s\right]\right.$$
$$\left. - 4 \cdot k_2 C(1-x)\right] + T_o = T.$$

26

MATLAB SCRIPT FOR OPTIMISING PARAMETERS AND MAXIMISING PROFIT FOR ADIABATIC CSTR IN PART 3.4:

```matlab
syms x s t %creating symbolic variables X, S and t for residence time for which to solve
V = 10*10^3; Q= 2500; d = 0.8; R = 8.314; ca0 = 1; H1 = -30*10^3; H2 = 40*10^3; %defining critical parameters
c = 100; %number of iterations for which answer is to be sought
cb0 = 1.993; %initial guess for optimal cb0
Ar1=4*10^6; Ar2=10^10; keq=2*10^-4; e1=50*10^3; e2=75*10^3;
T_out = linspace(298,363,c); %array for outlet temperature
X = zeros(1,c);
S = zeros(1,c);
XS = zeros(1,c);
time = zeros(1,c);
T0 = zeros(1,c);
Cc = zeros(1,c); %specifying number of iterations on each critical variable including defined objective function
profitability = zeros(1,c);


for i=1:c %loop for iterating over varying inlet temperature
    T = T_out(i);
    k1 = Ar1*exp(-e1/(R*T)); k2 = Ar2*exp(-e2/(R*T));   K = keq*exp(-H1/(R*T));
    options = optimoptions('fsolve','MaxFunctionEvaluations',100);
    fun = @(sol) [1-sol(2)-k2*(1-sol(1))*sol(3)/sol(1) ; -sol(2)+(k1*(1-sol(1))*cb0+k2*(1-sol(1))-
(sol(1)/sol(3)))/(sol(1)*(k1*(1-sol(1))*ca0+(k1/K))) ; -sol(3)+sol(1)*sol(2)/(k1*(1-sol(1))*(cb0-sol(1)*sol(2)*ca0)-
(k1*sol(1)*sol(2)/K))];
    sol0 = [0.5,0.5,150]; %solving equations derived from molar balances and later adding the third independent one
from energy balance for temperature
    sol = fsolve(fun,sol0,options);
    x = sol(1);
    s = sol(2);
    t = sol(3); %using matlab solver
    deltaT = (-(-k1*ca0*(1-x)*(cb0-x*s*ca0)+k1*x*s*ca0/K)*-H1+-k2*ca0*(1-x)*-H2)/(d*Q); %temperature equation from
energy balance

    X(i) = x;
    S(i) = s;
    XS(i) = x*s;
    time(i) = t;
```

```matlab
        T0(i) = T - deltaT;
        Cc(i) = ca0*x*s*V/t; %concentration of C
        negative = (5*ca0+cb0)*V/t; %objective function costs
        income = (10*ca0*x*s+4.5*ca0*(1-x))*V/t; %objective function income
        profits = (income-negative)*60;
        if profits > 0.001 && Cc(i) > 50
            profitability(i) = profits; %adding and assigning constraint based on Cc
        else
            profitability(i) = 0; %preventing appearance of non physical solutions
        end
    end
end
[Val,Idx] = max(profitability);
Peak = Val
Conversion = X(Idx)
Selectivity = S(Idx)
Residence_time = time(Idx) %displaying optimal values
```