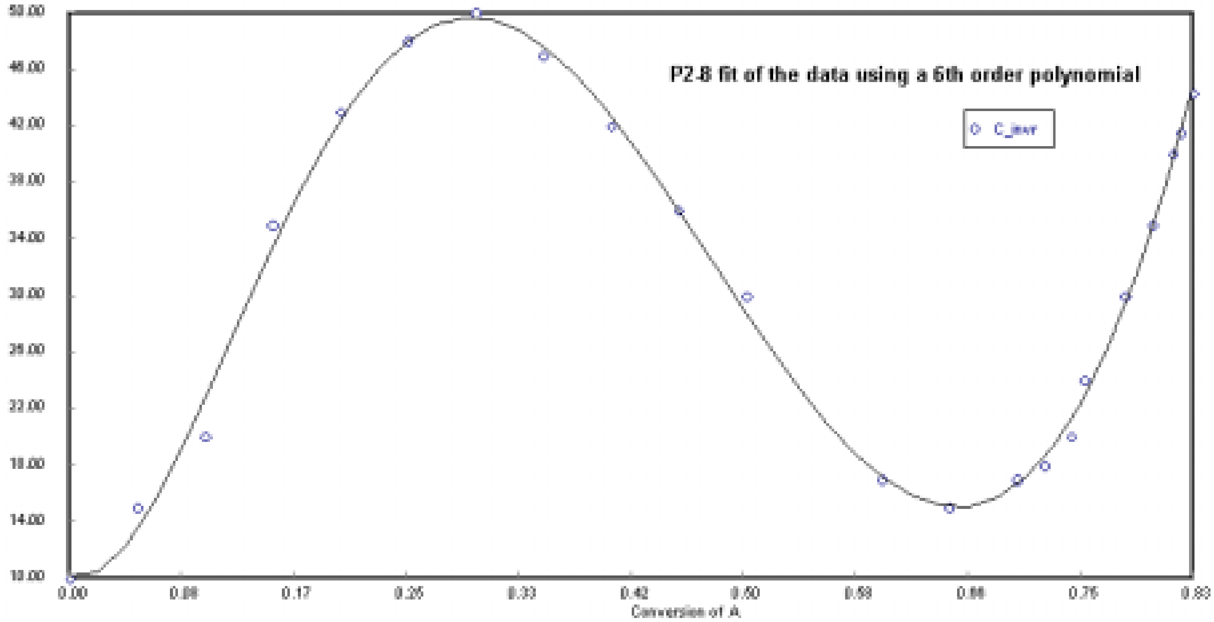
Data for Problem 2-8a
From manual Digitization of the Graph of Figure P2-8a

conversion	C_invr
0	10
0.05	15
0.1	20
0.15	35
0.2	43
0.25	48
0.3	50
0.35	47
0.4	42
0.45	36
0.5	30
0.6	17
0.65	15
0.7	17
0.72	18
0.74	20
0.75	24
0.78	30
0.8	35
0.815	40
0.8212	41.5
0.83	44.29

A fit of the data using a 6th order regression gives:



POLYMATH Results

Problem 2-8 Reactor Sequencing 02-04-2002

Polynomial Regression Report

Model: C_invr = a0 + a1*conv + a2*conv^2 + a3*conv^3 + a4*conv^4 + a5*conv^5 + a6*conv^6

Variable	Value	95% confidence
a0	10.275793	2.3998253
a1	-42.690176	91.985097
a2	2639.4645	1066.5262
a3	-1.128E+04	5025.2971
a4	1.842E+04	1.117E+04
a5	-1.356E+04	1.17E+04
a6	3981.0814	4650.1117

General
Order of polynomial = 6
Regression including free parameter
Number of observations = 22

Statistics

R^2 =	0.9940911
R^2adj =	0.9917275
Rmsd =	0.2037993
Variance =	1.3401686

Fit using Excel:

conv	C_invr	datafit	polymath data fit	excel data fit
0	10	10.27579	10.27579	10.27579
0.05	15	13.44144	13.4409	13.44144
0.1	20	22.83598	22.8318	22.83598
0.15	35	33.54438	33.53098	33.54438
0.2	43	42.49384	42.46393	42.49385
0.25	48	48.05714	48.00266	48.05715
0.3	50	49.70069	49.61395	49.7007
0.35	47	47.67742	47.55238	47.67744
0.4	42	42.76449	42.59815	42.76452
0.45	36	36.04568	35.83973	36.04572
0.5	30	28.73867	28.50123	28.73873
0.6	17	17.17727	16.93664	17.17736
0.65	15	15.09991	14.91071	15.10003
0.7	17	16.75644	16.67332	16.7566
0.72	18	18.65796	18.63644	18.65814
0.74	20	21.34995	21.40282	21.35015
0.75	24	23.0102	23.10546	23.0104
0.78	30	29.33855	29.58391	29.33878
0.8	35	34.76241	35.12873	34.76266
0.815	40	39.51405	39.98317	39.51432
0.8212	41.5	41.65821	42.17302	41.65849
0.83	44.29	44.88954	45.47254	44.88982

Notice that the data in the column *polymath data fit* (in red) is different than that calculated by polymath. This error is caused by a loss of significant digits in using the POLYMATH data fit equation. The values calculated by POLYMATH have the full set of significant digits, but the equations are limited to 4 significant digits in scientific notation.

$v_0 = 50$ L/min find V= total

for a PFR at ss

$$\frac{dF_A}{dV} = r_A \qquad X_A = \frac{F_{A0} - F_A}{F_{A0}}$$

$$F_A = F_{A0} - X_A F_{A0}$$
$$dF_A = 0 - F_{A0} X_A$$

$$-F_{A0}\frac{dX_A}{dV} = r_A$$

$$\tau = \frac{V}{v_0} \qquad v_0 = v$$ since it is a liquid ($\rho_0 = \rho$)

$$dV = v_0 \, d\tau$$

$$-\frac{F_{A0}}{v_0}\frac{dX_A}{d\tau} = r_A$$

$$C_{A0} = F_{A0}/v_0 \quad \frac{\text{mol A}}{\text{min}}\,\frac{\text{min}}{\text{L}}$$

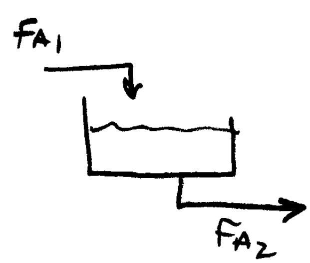
$$\tau = \int d\tau = -\int \frac{C_{A0}}{r_A}\, dX_A$$

Using a numerical integration package in Polymath

$$\text{for} \quad -\int_0^{0.3} \frac{C_{A0}}{r_A} dX_A = 9.58 \text{ min}$$

$$V_{PFR} = 50 \frac{\text{L}}{\text{min}} \, 9.58 \text{min} = 479 \text{ L}$$

For the CSTR



well-mixed
V_2 = C.V.

$$0 = F_{A1} - F_{A2} + r_{A2} V_2$$

$$F_{A1} = F_{A0} - F_{A0} X_{A1}$$
$$F_{A2} = F_{A0} - F_{A0} X_{A2}$$

$$F_{A1} - F_{A2} = 0 - F_{A0} X_{A1} + F_{A0} X_{A2}$$

$$0 = -F_{A0}X_{A_1} + F_{A0}X_{A_2} + r_{A_2}V$$

$$\frac{-F_{A0}(X_{A_2} - X_{A_1})}{r_{A_2}} = V \quad \leftarrow \quad \left\{ F_{A0} = C_{A0}/v_0, \quad \tau = \frac{V}{v_0} \right.$$

$$-\frac{C_{A0}}{r_{A_2}}(X_{A_2} - X_{A_1}) = \tau$$

Find $\frac{C_{A0}}{-r_{A_2}}$ at $X_{A_2} = 0.7$

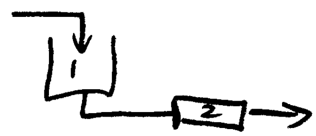
from table $\frac{C_{A0}}{-r_{A_2}} = 17\text{ min}$

$$\tau_2 = (17\text{min})(0.7 - 0.3) = 6.8\text{min}$$

$$V_2 = v_0\tau_2 = 50\frac{L}{\text{min}}\ 6.8\text{min} = 340L$$

$$\boxed{V_T = V_1 + V_2 = 479 + 340 = 819L}$$

Note for the other scheme:



$$\tau = -\frac{C_{A0}}{r_{A_1}}(X_{A_1} - 0)$$

$$= -50\text{min}(0.3) = 15\text{min}$$

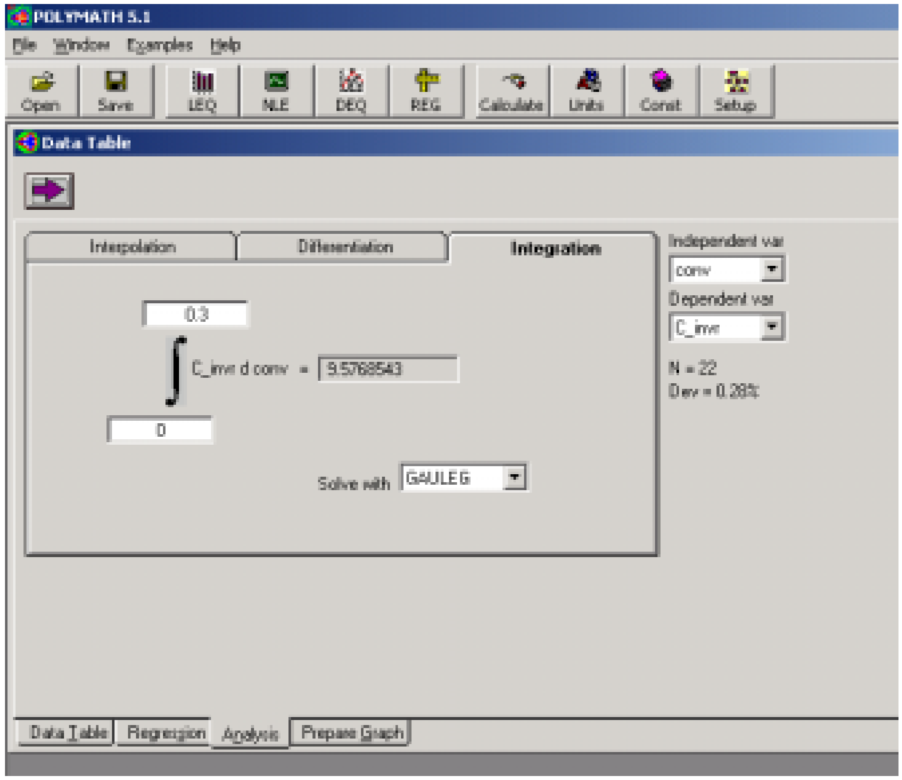
$$V_1 = 50L/\text{min}\ 15\text{min} = 750L$$

and for PFR

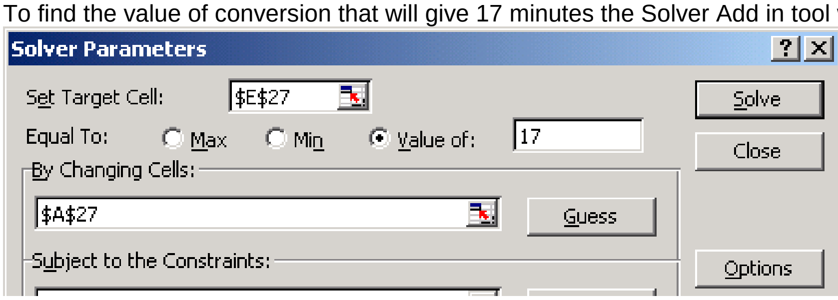
$$\tau_2 = \int_{0.3}^{0.7} -\frac{C_{A0}}{r_A}dx = 12.15\text{min} \qquad V_2 = 50\frac{L}{\text{min}}\ 12.15\text{min} = 607.5L$$

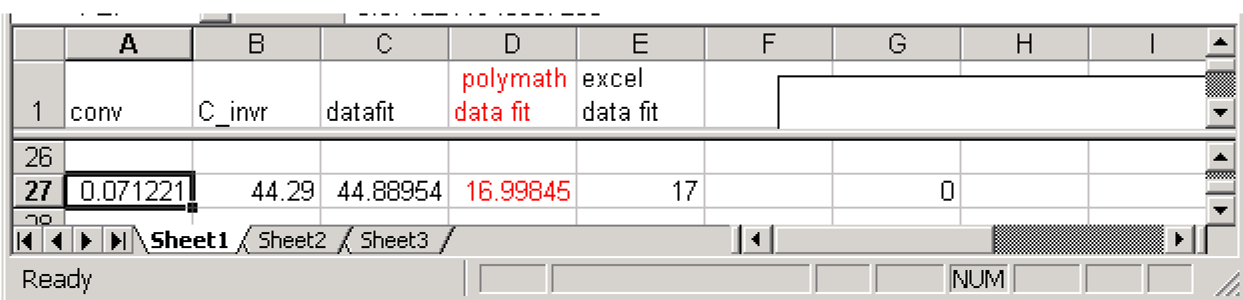
$V_T = 1358L$ this value is much larger than 819L

Reactor Sequence: PFR followed by CSTR
The following was obtained for the PFR:

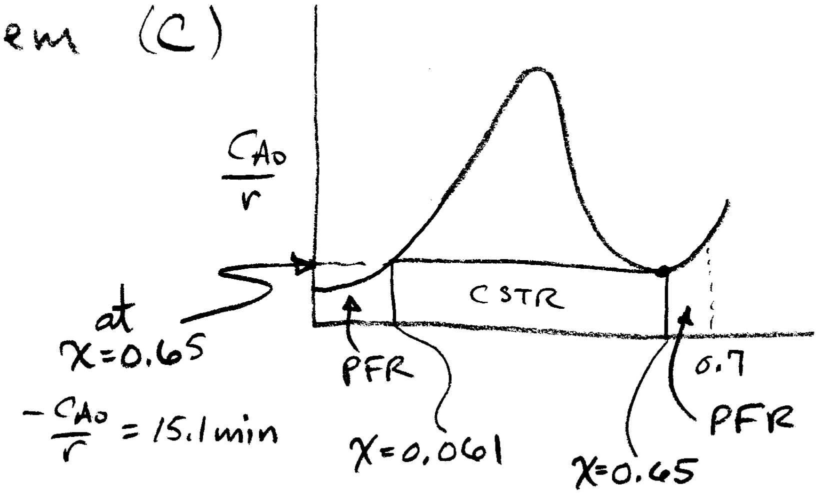


To find the value of conversion that will give 17 minutes the Solver Add in tool will be used.





Problem (C)



$$\tau_{CSTR} = -\frac{C_{A0}}{r}\left(X_2 - X_1 \right) = (15.1\,\text{min})(0.65 - 0.061)$$

$$= 8.9\,\text{min}$$

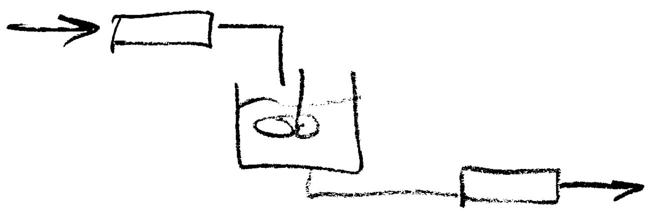
$$V_{CSTR} = 8.9\,\text{min}\ \frac{50\,L}{\text{min}} = 445\,L$$

$$\tau_{PFR1} = \int_0^{0.06} \frac{C_{A0}}{-r}\,dX = 0.79\,\text{min}$$ using Polymath integration

$$\tau_{PRR2} = \int_{0.65}^{0.7} \frac{C_A}{-r}\,dX = 0.79\,\text{min}$$ " "

$$V_{PRR1} = V_{PFR2} = 0.79\,\text{min}\ (50\ L/\text{min}) = 39.5\,L$$

$$V_{Total} = 2(39.5\,L) + 445\,L = 524\,L$$



V = 524L

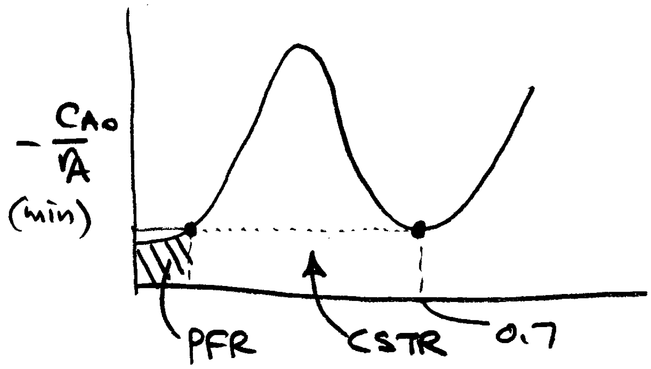
If one PFR followed by a CSTR is used then

V = 582 L

see next page

c) Is there a smaller volume for a reactor sequence to achieve $X_A = 0.7$?

The Ideal sequence is to use a PFR followed by a CSTR



PFR would end at $\left.\frac{C_{A0}}{-r_A}\right|_{X_A=\text{small}} = \left.\frac{C_{A0}}{r_A}\right|_{X_A=0.7} =$

from Table

$$\left.C_{A0}/r_A\right|_{X_A=0.7} = 17 \text{ min}$$

A similar value is found in the range $0.05 < X_A < 0.1$

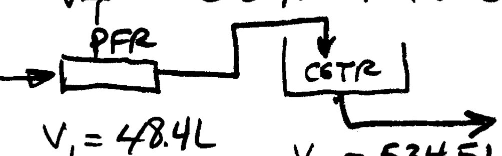
Using the solver add-in tool

$$X_A = 0.0712 \quad \text{for} \quad C_{A0}/r_A = 17\text{min}$$

$$\tau_1 = \int_0^{0.0712} \frac{C_{A0}}{-r_A}\,dX = 0.967 \text{ min} \qquad V_1 = \frac{50L}{min}\,0.967 = 48.35L$$

$$\tau_2 = (17\text{min})(0.7 - 0.0712) = 10.7\text{min} \qquad V_2 = 10.7\text{min}\,\frac{50L}{min} = 534.5$$

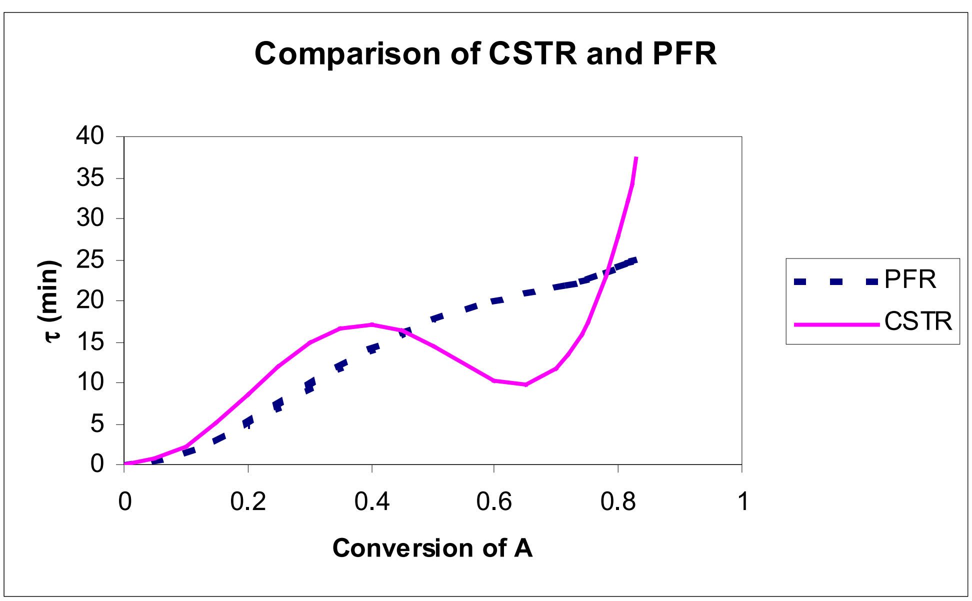
$$V_T = 534.5 + 48.35L = 582.35L$$

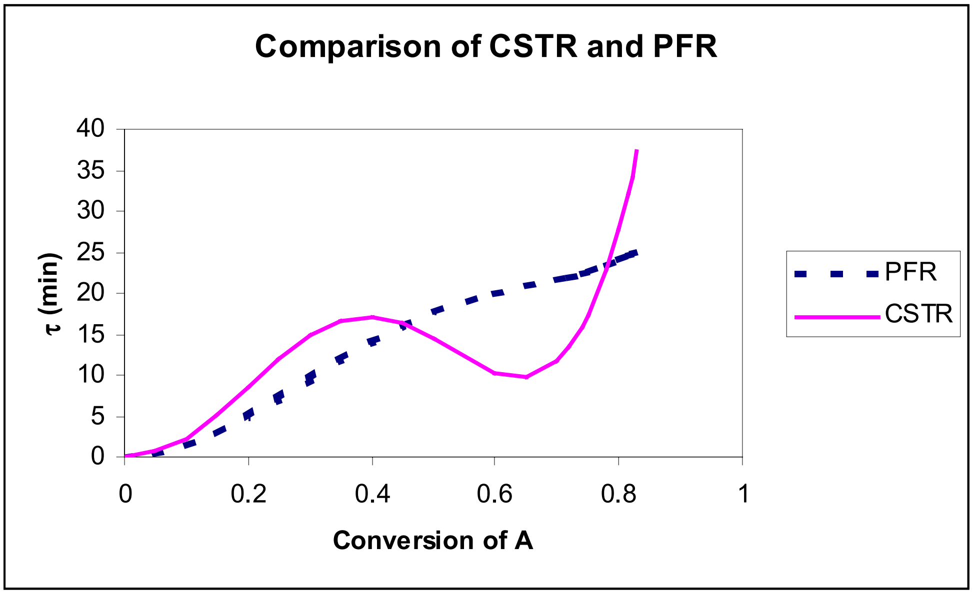


$$\boxed{V_T = 582L}$$

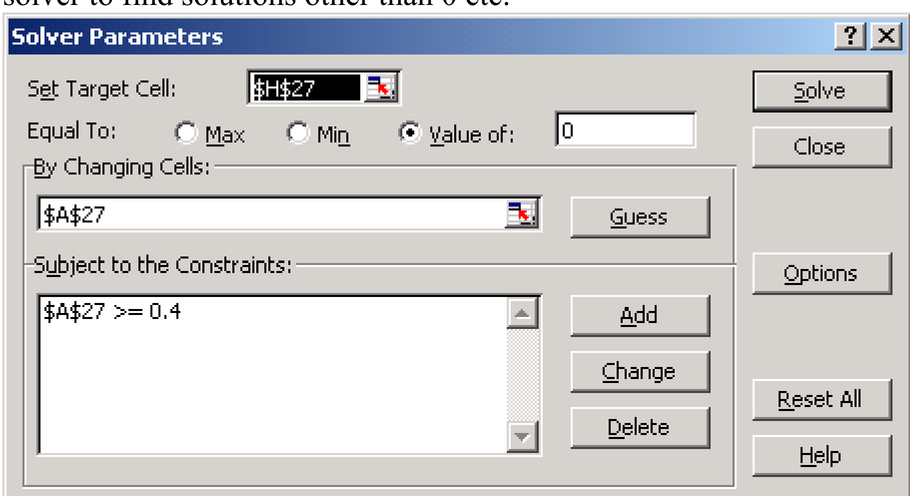
(d) The solution for this problem was found by integrating the polynomial expression for conversion divided by reaction rate for the PFR. The plug flow reactor equation was integrated and a new column was created with title Tau for PFR: = 3981.0815*conv^7/7 - 13564.306*conv^6/6 + 18416.881*conv^5/5 - 11275.464*conv^4/4 + 2639.4645*conv^3/3 - 42.690177*conv^2/2 + 10.275793*conv

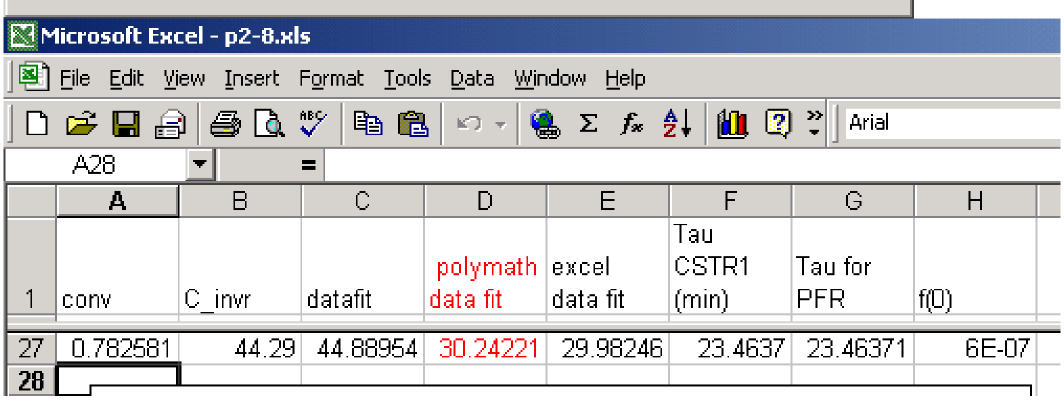
conv	C_invr	datafit	polymath data fit	excel data fit	Tau CSTR1 (min)	Tau for PFR
0	10	10.27579	10.27579	10.27579	0	0
0.05	15	13.44144	13.4409	13.44144	0.672072	0.553903
0.1	20	22.83598	22.8318	22.83598	2.283598	1.446693
0.15	35	33.54438	33.53098	33.54438	5.031657	2.858378
0.2	43	42.49384	42.46393	42.49385	8.498769	4.771016
0.25	48	48.05714	48.00266	48.05715	12.01429	7.050722
0.3	50	49.70069	49.61395	49.7007	14.91021	9.510967
0.35	47	47.67742	47.55238	47.67744	16.6871	11.95939
0.4	42	42.76449	42.59815	42.76452	17.10581	14.23038
0.45	36	36.04568	35.83973	36.04572	16.22057	16.20567
0.5	30	28.73867	28.50123	28.73873	14.36936	17.82515
0.6	17	17.17727	16.93664	17.17736	10.30642	20.06163
0.65	15	15.09991	14.91071	15.10003	9.815022	20.85486
0.7	17	16.75644	16.67332	16.7566	11.72962	21.6339
0.72	18	18.65796	18.63644	18.65814	13.43386	21.98678
0.74	20	21.34995	21.40282	21.35015	15.79911	22.3855
0.75	24	23.0102	23.10546	23.0104	17.2578	22.60712
0.78	30	29.33855	29.58391	29.33878	22.88425	23.38715
0.8	35	34.76241	35.12873	34.76266	27.81013	24.02649
0.815	40	39.51405	39.98317	39.51432	32.20417	24.5828
0.8212	41.5	41.65821	42.17302	41.65849	34.20995	24.83438
0.83	44.29	44.88954	45.47254	44.88982	37.25855	25.21503





Using the Solver Add-in Tool the space times and conversions were identified. Notice that in using the Solver a constraint can be placed on the solution to restrict values. For example to find the solution around 0.45 a constraint was added requiring that $\chi_A \geq 0.4$. This will force the solver to find solutions other than 0 etc.





d) $\tau_{CSTR} = \tau_{PFR}$ or $V_{CSTR} = \tau_{PFR}$

$$\tau_{CSTR} = -\frac{C_{A0}}{r_A}\left(\chi_{A_{CSTR}} - 0\right) = \int_0^{\chi_{A\,PFR}} -\frac{C_{A0}}{r_A}\, d\chi_A = \tau_{PFR}$$

Find the possible conversions

Integrating a Polynomial:

$$\int (a + bx + cx^2 + dx^3 + ex^4 + fx^5 + gx^6)\, dx$$

$$= ax + b\frac{x^2}{2} + c\frac{x^3}{3} + \frac{dx^4}{4} + \frac{ex^5}{5} + f\frac{x^6}{6} + g\frac{x^7}{7} \Big|_{x=0}^{x}$$

Now putting this formula into a spreadsheet or Polymath call and plotting shows that there are 4 solutions (including 0=0)

By Trial & error – using the solver the following answers are obtained:

$\tau_{CSTR} = \tau_{PFR}$	$\chi_{CSTR} = \chi_{PFR}$
0	0
0.13 min	0.013
16.2 min	0.45
23.5 min	0.783

← this point (0.013) may only be a result of the 6th order polynomial fit.

See graph on Next Page

(e)

Plot of τ_{CSTR} vs X

for $V = 700L$ and $v_0 = 50 L/min$

$X = ?$

$$\tau = \frac{700 L}{50 L/min} = 14.0 min$$

The curve shows that there are 3 solutions

Using the root finder will give the answer:

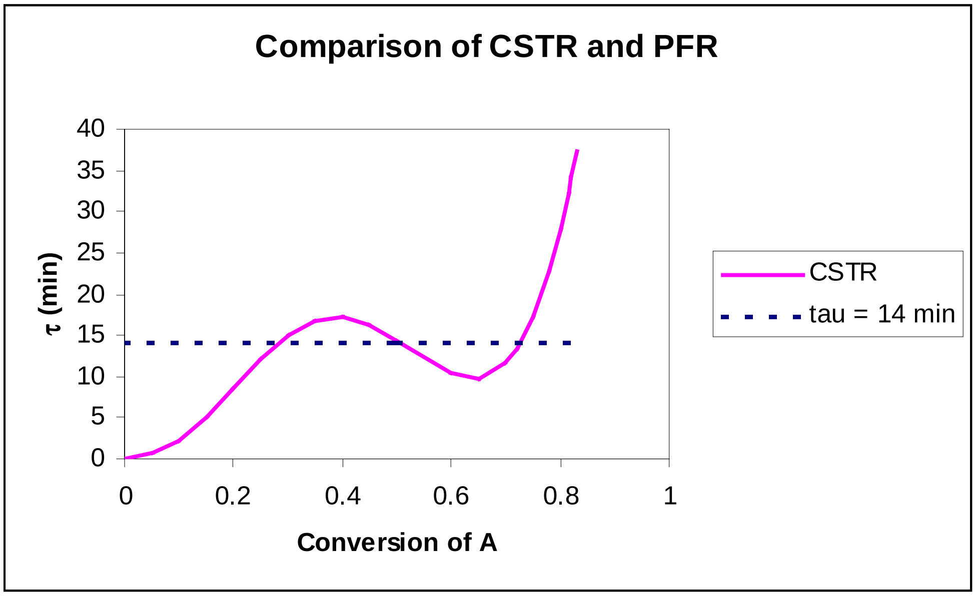
$\tau = 14 min$

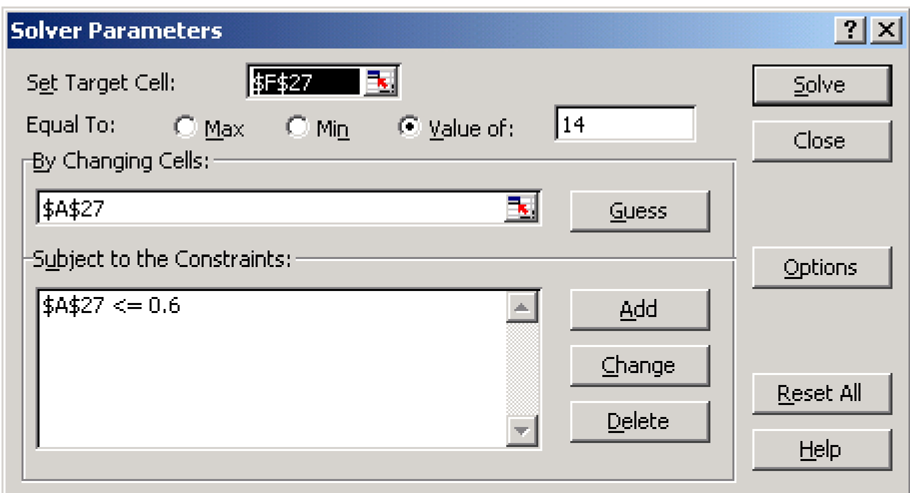
CSTR
- $X = 0.282$
- $X = 0.51$ — used constraint $X \leq 0.6$
- $X = 0.725$ — used constraint $X \geq 0.6$

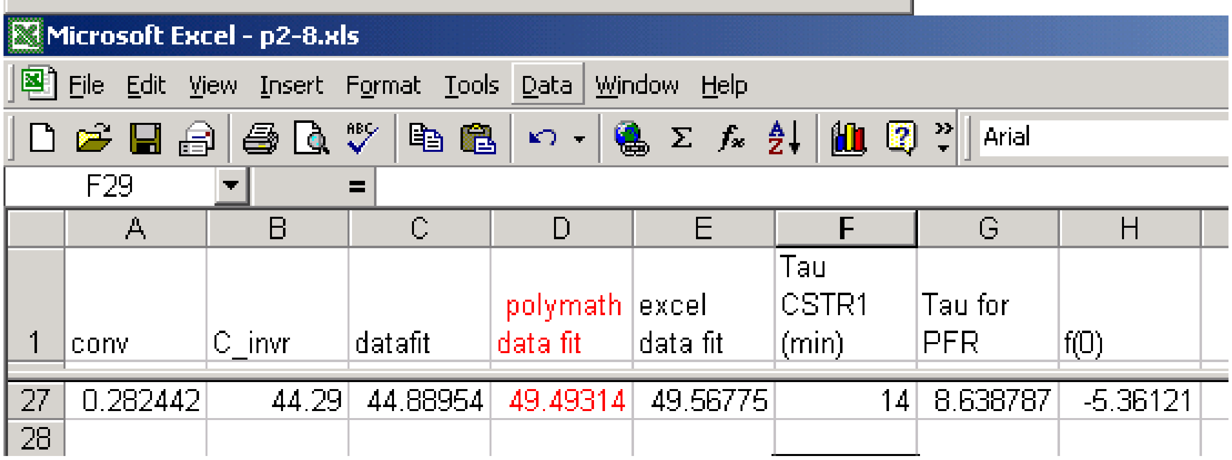
10:43

2hr 15min

Part (e)


Comparison of CSTR and PFR
τ (min)
40
35
30
25
20
15
10
5
0
0
0.2
0.4
0.6
0.8
1
Conversion of A
CSTR
tau = 14 min


Solver Parameters
Set Target Cell:
F27
Equal To:
Max
Min
Value of:
14
By Changing Cells:
A27
Guess
Subject to the Constraints:
A27 <= 0.6
Add
Change
Delete
Solve
Close
Options
Reset All
Help


Microsoft Excel - p2-8.xls
File Edit View Insert Format Tools Data Window Help
Arial
F29
=
A B C D E F G H
1 conv C_invr datafit polymath data fit excel data fit Tau CSTR1 (min) Tau for PFR f(0)
27 0.282442 44.29 44.88954 49.49314 49.56775 14 8.638787 -5.36121
28