Workshop 02 Solution: Conversion and reactor sizing

Lecture notes for chemical reaction engineering

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Problem 1

P2-3: You have two CSTRs and two PFRs, each with a volume of $1.6 m^3$. Use Figure 1 to calculate the conversion for each of the reactors in the following arrangements.

(a) Two CSTRs in series.
(b) Two PFRs in series.
(c) Two CSTRs in parallel with the feed, F_{A0}, divided equally between the two reactors.
(d) Two PFRs in parallel with the feed divided equally between the two reactors.
(e) A CSTR and a PFR in parallel with the flow equally divided. Calculate the overall conversion, X_{ov}

$$X_{ov} = \frac{F_{A0} - F_{A,CSTR} - F_{A,PFR}}{F_{A0}}$$

with

$$F_{A,CSTR} = \frac{F_{A0}}{2} - \frac{F_{A0}}{2} X_{CSTR}, \text{and } F_{A,PFR} = \frac{F_{A0}}{2}(1 - X_{PFR})$$

(f) A PFR followed by a CSTR.
(g) A CSTR followed by a PFR.
(h) A PFR followed by two CSTRs. Is this arrangement a good arrangement or is there a better one?

Solution:

To read the CSV file use the `genfromtxt` function from numpy

```
import numpy as np

p1_expt_file = './workshop-02-problem-1-data.csv'
p1_expt_data = np.genfromtxt(p1_expt_file,
                             delimiter=',',
                             dtype=[('x', float),
                                    ('fa0_by_ra', float)],
                             skip_header=1)
```

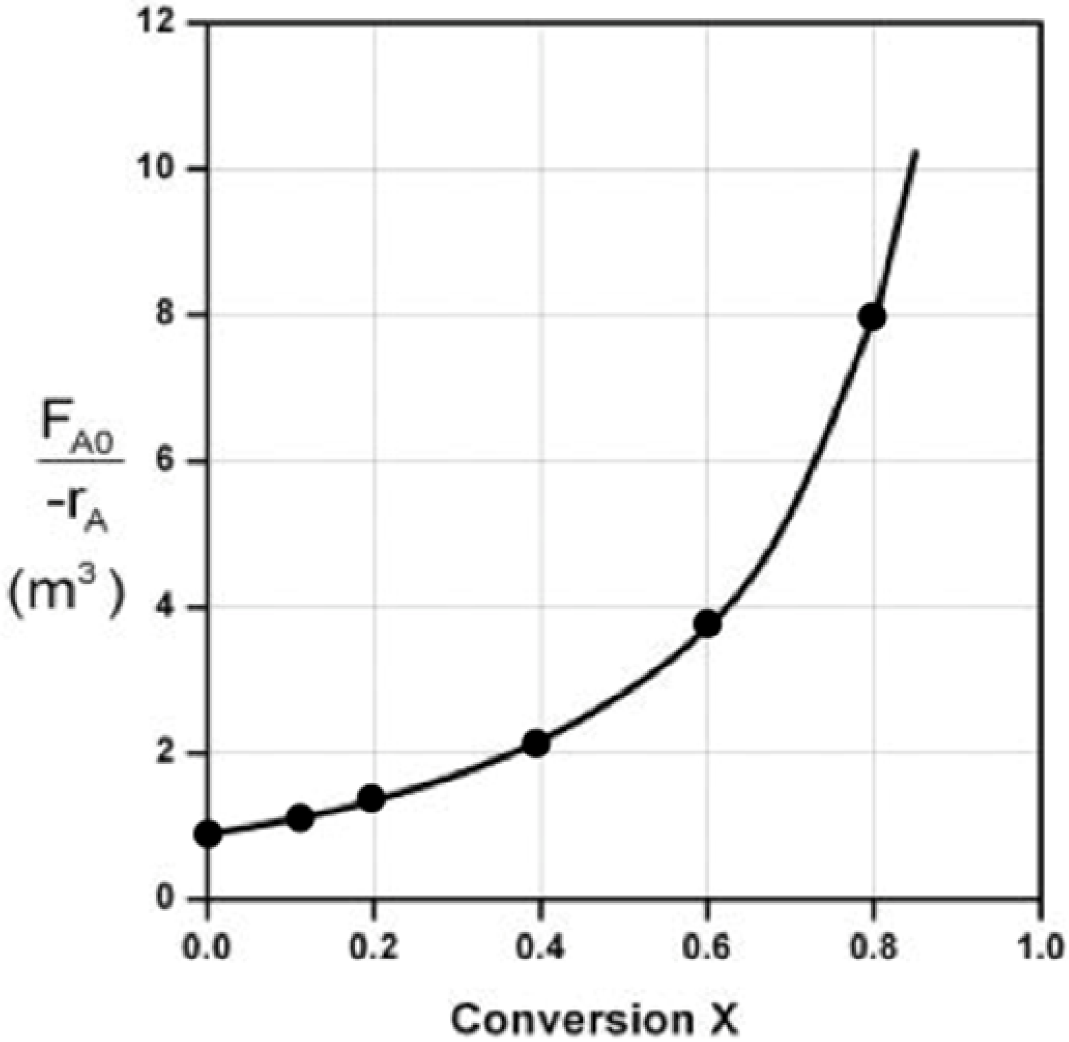

Figure 2-2B Levenspiel plot of processed data 2.

Figure 1: Figure-2-2b

To interpolate the data, use `CubicSpline` function from `scipy.interpolate`.

```
import scipy.interpolate as interpolate

p1_interp = interpolate.CubicSpline(p1_expt_data['x'],
                                    p1_expt_data_data['fa0_by_ra'])
```

Data plotting using `matplotlib.pyplot`

```
import matplotlib.pyplot as plt

fig,ax = plt.subplots()

ax.scatter(p1_expt_data['x'],
           p1_expt_data['fa0_by_ra'],
           marker='s',
           color='red')

ax.set_xlabel('Conversion X')
ax.set_ylabel('$\\frac{F_{A0}}{-r_A} (m^3)$')

# Setting x and y axis limits
ax.set_xlim(0, 1)
ax.set_ylim(0, 12)

plt.show()
```

Add fit line to the plot

```
x_interp =np.linspace(0,1,100)
ax.plot(x_interp, p1_interp(x_interp), color='grey')
```

Add rectangle to the plot

```
# Adds rectangle from (0,0) with a width of x1 and height of y1
rectangle = plt.Rectangle((0, 0), x1, y1, color='skyblue', alpha=0.4)
ax.add_patch(rectangle)
```

Color area under the curve

```
 Fill the area under the curve between x1 and x2
x_fill = np.linspace(x1, x2, 100)
y_fill = p1_interp(x_fill)
ax.fill_between(x_fill, y_fill, color='skyblue', alpha=0.4)
```

(a) Two CSTRs in series (Figure 3).

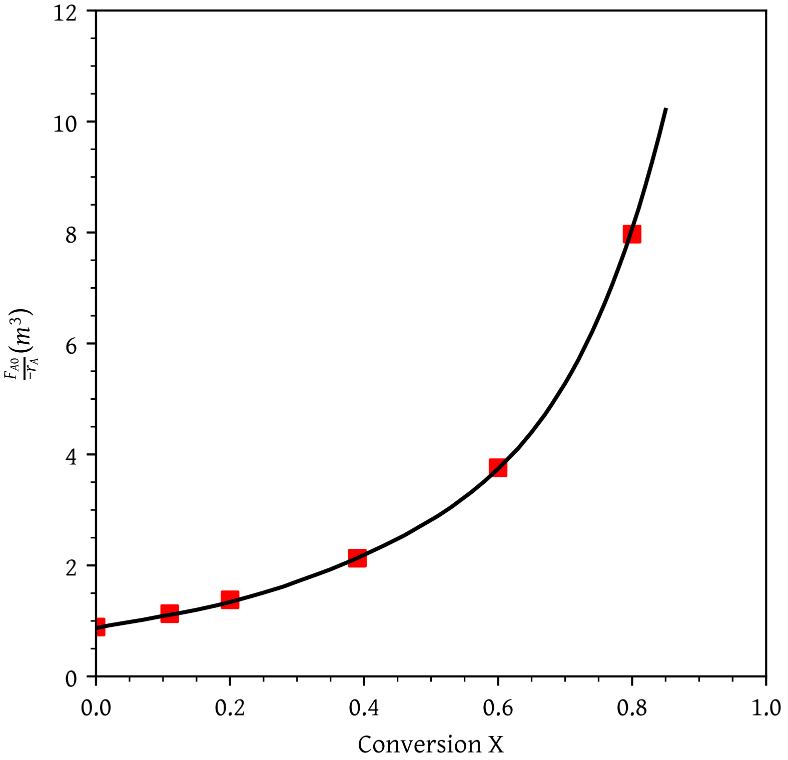

Figure 2: Levenspiel plot of processed data 2 for problem 2-2b

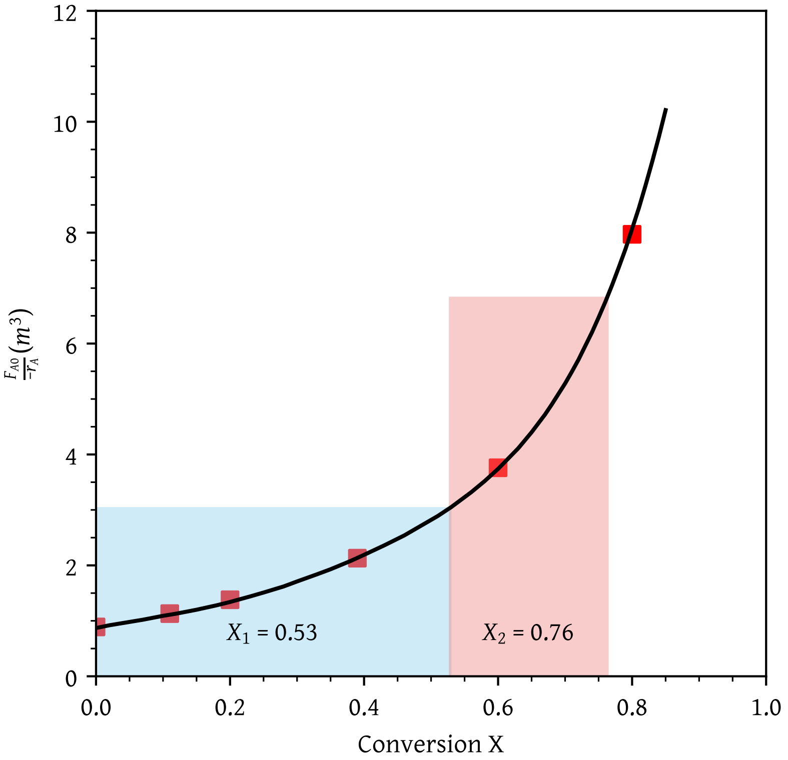

Figure 3: Conversion from two CSTR in series

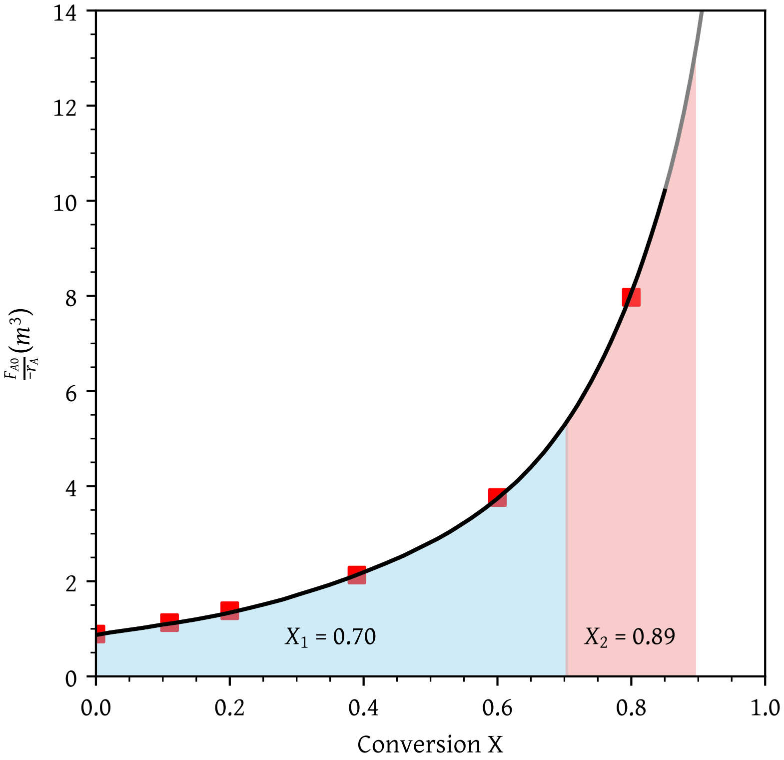

Figure 4: Conversion from two PFR in series

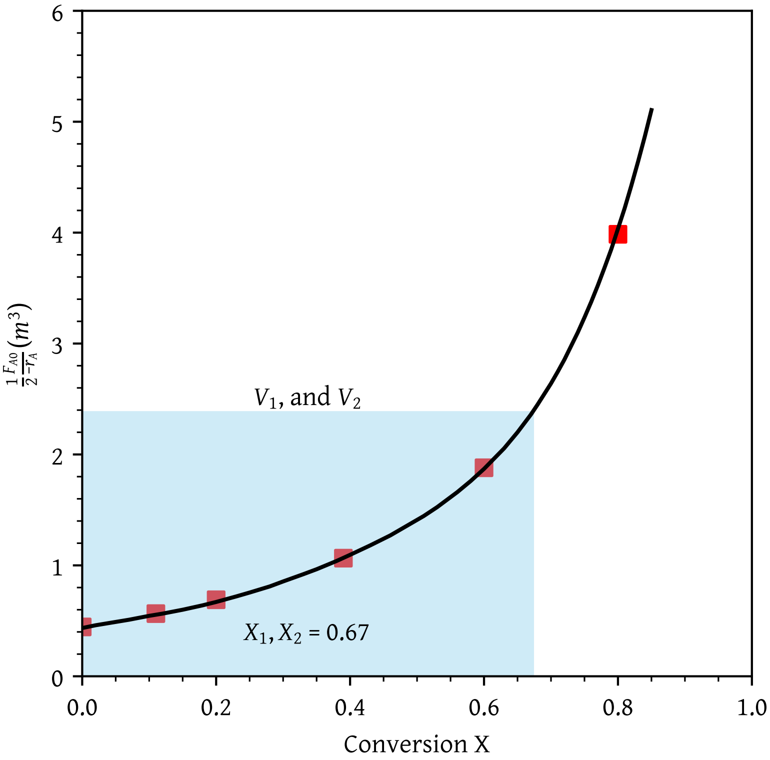

Figure 5: Conversion from two CSTR in parallel

(b) Two PFRs in series (Figure 4).

(c) Two CSTRs in parallel with the feed, F_{A0}, divided equally between the two reactors (Figure 5).

(d) Two PFRs in parallel with the feed divided equally between the two reactors (Figure 6).

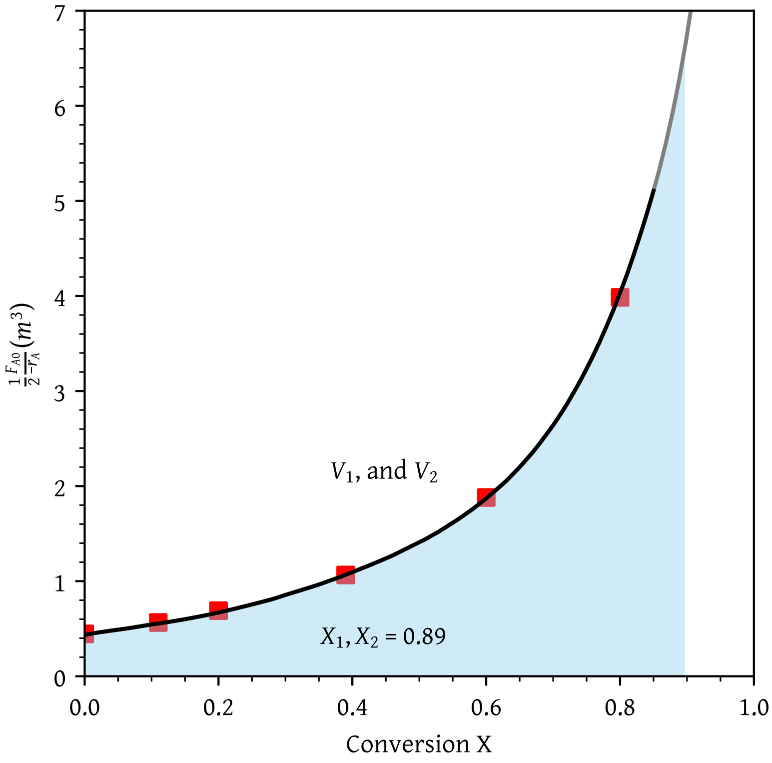

Figure 6: Conversion from two PFR in parallel

(e) A CSTR and a PFR in parallel with the flow equally divided. Calculate the overall conversion, X_{ov} (Figure 7)

(f) A PFR followed by a CSTR (Figure 8).

(g) A CSTR followed by a PFR (Figure 9).

(h) A PFR followed by two CSTRs (Figure 10). Is this arrangement a good arrangement or is there a better one?

Two CSTRs followed by a PFR (Figure 11) yield final conversion of X_3 = 0.92.

Two PFRs followed by a CSTR (Figure 12) yield final conversion of X_3 = 0.97.

Problem 2

P2-4: The exothermic reaction of stillbene (A) to form the economically important trospophene (B) and methane (C), i.e.,

$$\mathrm{A} \longrightarrow \mathrm{B} + \mathrm{C}$$

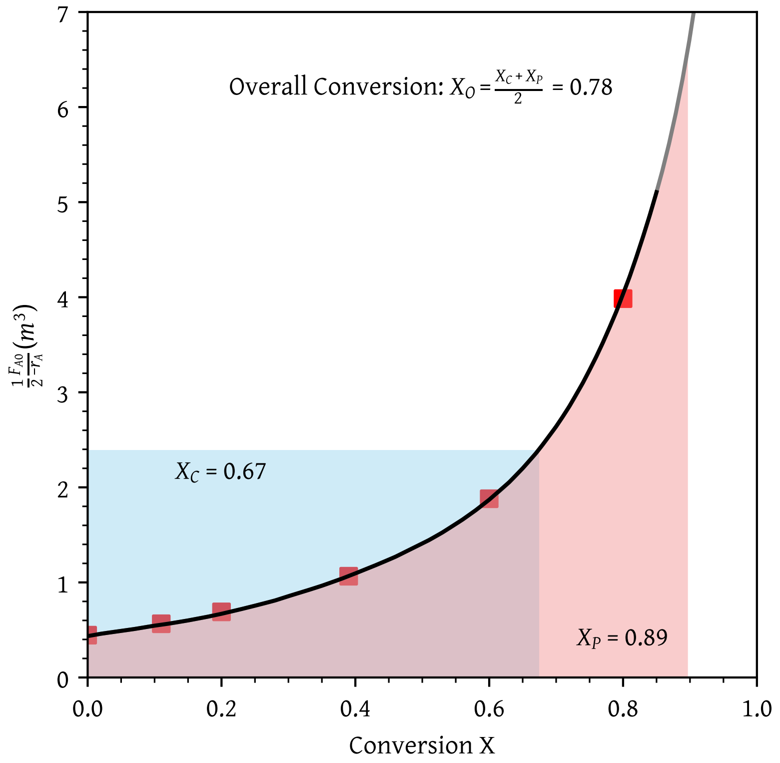

Figure 7: Conversion from a CSTR and a PFR in parallel

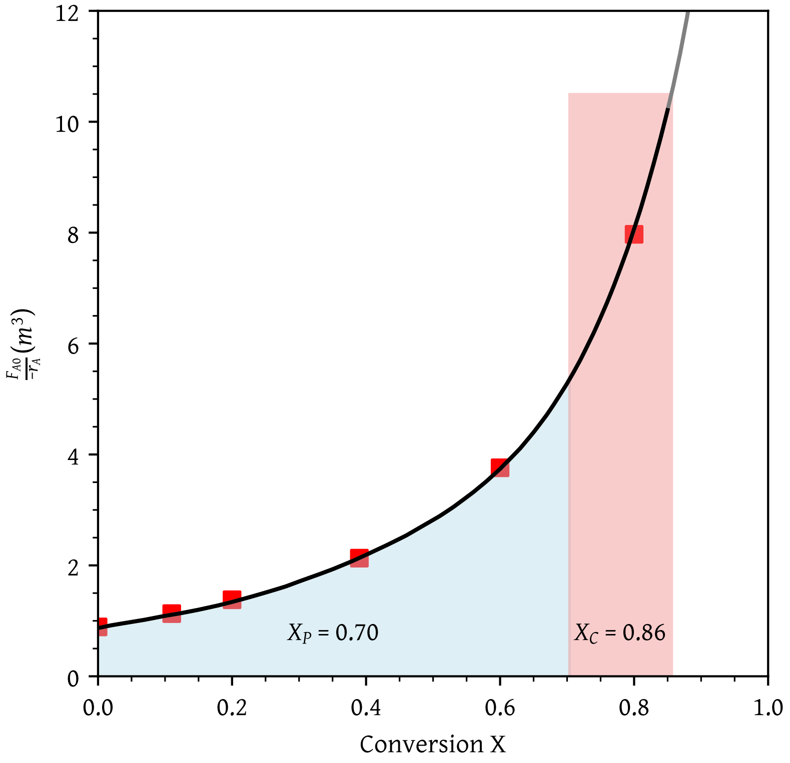

Figure 8: Conversion from a PFR followed by CSTR

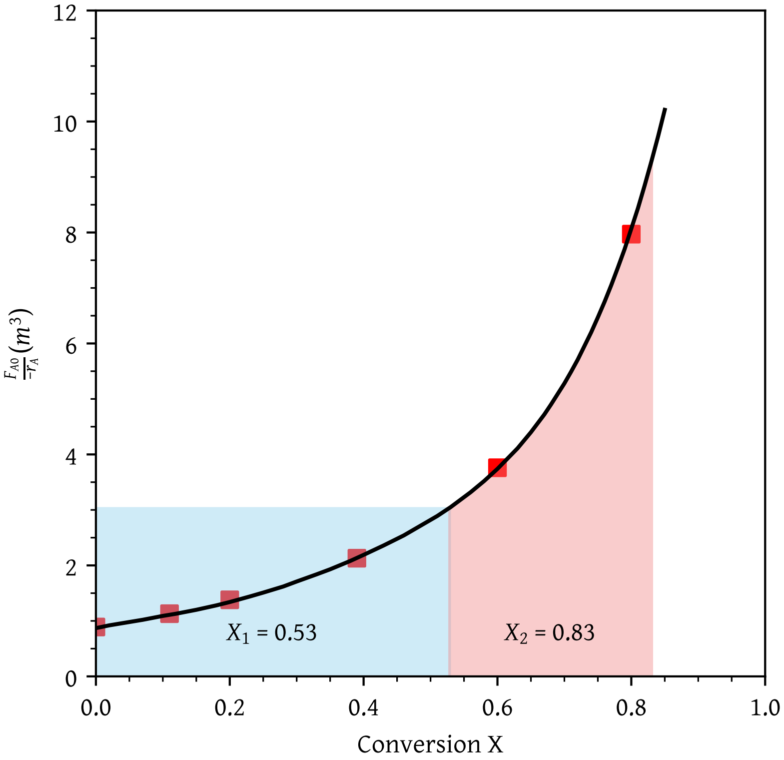

Figure 9: Conversion from a CSTR followed by PFR

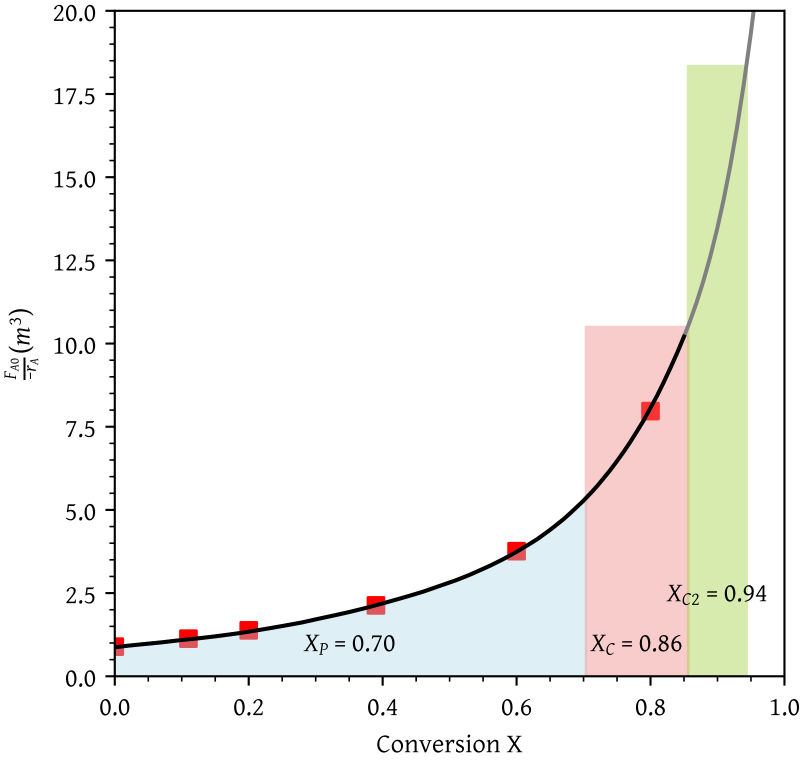

Figure 10: Conversion from a PFR followed by two CSTRs

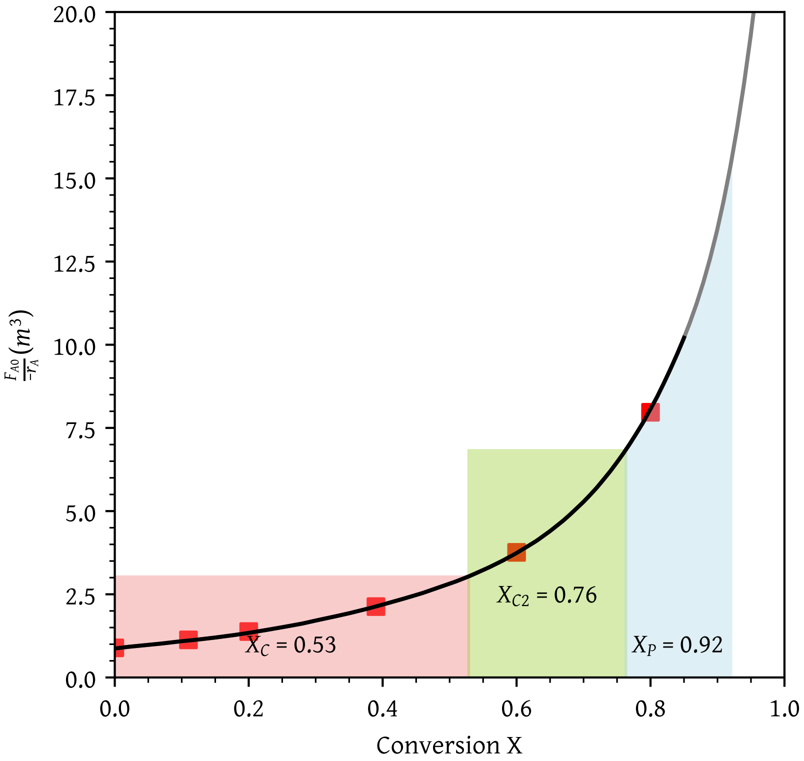

Figure 11: Conversion from two CSTRs followed by a PFR

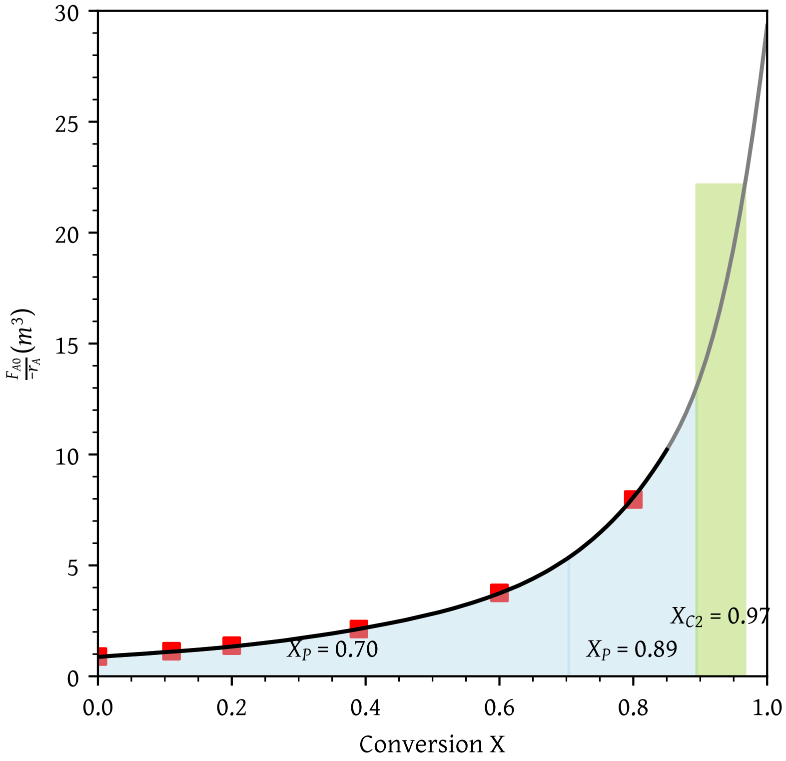

Figure 12: Conversion from two PFRs followed by a CSTR

was carried out adiabatically and the following data recorded:

Table 1: Problem 2.4 rate data

X	$-r_A (mol/dm^3 min)$
0	1
0.2	1.67
0.4	5
0.45	5
0.5	5
0.6	5
0.8	1.25
0.9	0.91

The entering molar flow rate of A was $300 mol/min$.

(a) What are the PFR and CSTR volumes necessary to achieve 40% conversion?
(b) Over what range of conversions would the CSTR and PFR reactor volumes be identical?
(c) What is the maximum conversion that can be achieved in a $105 dm^3$ CSTR?
(d) What conversion can be achieved if a $72 dm^3$ PFR is followed in series by a $24 dm^3$ CSTR?
(e) What conversion can be achieved if a $24 dm^3$ CSTR is followed in a series by a $72 dm^3$ PFR?
(f) Plot the conversion and rate of reaction as a function of PFR reactor volume up to a volume of $100 dm^3$.

Solution:

The rate data ($-r_A$) is given. We need $F_{A0}/-r_A$. Dividing $F_{A0} = 300$ by $-r_A$ we get:

Table 2: Processed data for problem 2

X	$-r_A$	$F_{A0}/-r_A$
0	1	300
0.2	1.67	179.641
0.4	5	60
0.45	5	60
0.5	5	60
0.6	5	60
0.8	1.25	240
0.9	0.91	329.67

Trying to fit a single cubic spline or a polynomial doesn't work well due to the nature of the data (Figure 13). The data consists of three liniear segments. Therefore, we fit a piecewise linear function using `numpy.piecewise`. We also use `lambda` functions to define the linear segments.

```
def piecewise_linear_fit(x, x0, y0, k1, k2, k3):
    """
    Piecewise linear function defined by slopes and a constant part.
    x0, y0: Coordinates of the piecewise function's bending points.
    k1, k2, k3: Slopes of the first, second, and third parts.
```

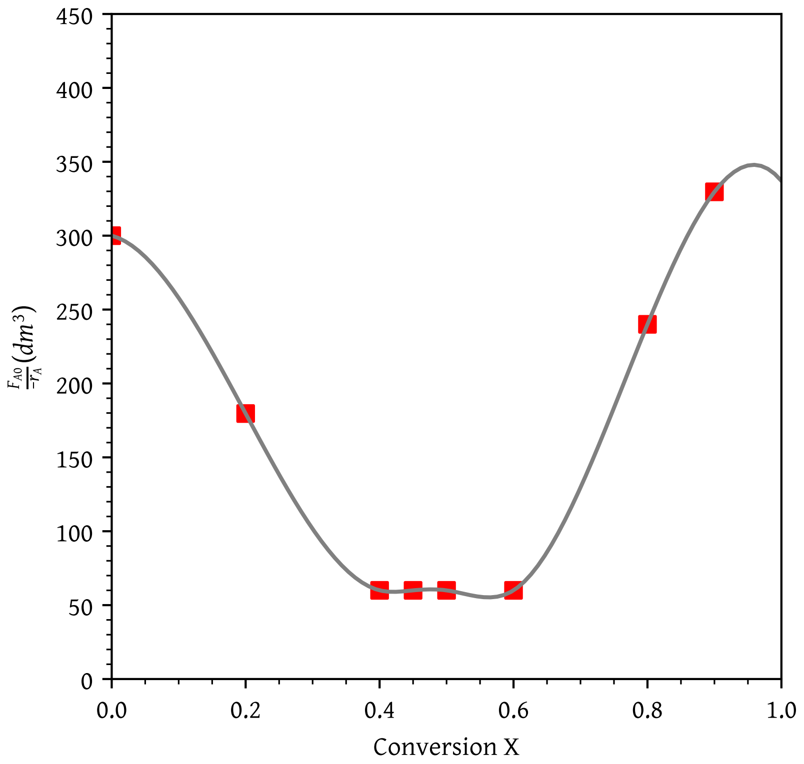

Figure 13: Levenspiel plot of processed data for problem 2-4

```
    Note that in this problem,
    k1 = -600.0
    k2 = 0
    k3 = 898.9010989010986

    x0 = [0.4, 0.6]
    y0 = [60.0, 60.0]

    We can call this function as
    piecewise_linear_fit(x, *args)

    args = ([0.4, 0.6], [60.0, 60.0], -600.0, 0, 898.9010989010986)
    """

    return np.piecewise(x,
                        [x < x0[0], (x >= x0[0]) & (x <= x0[1]), x > x0[1]],
                        [lambda x: k1*x + y0[0] - k1*x0[0],
                         lambda x: y0[1],
                         lambda x: k3*x + y0[1] - k3*x0[1]])
```

(a) What are the PFR and CSTR volumes necessary to achieve 40% conversion?

```
From @fig-problem-2a, $V_{CSTR}$ = 24\.00 $dm^3$.
```

(b) Over what range of conversions would the CSTR and PFR reactor volumes be identical?

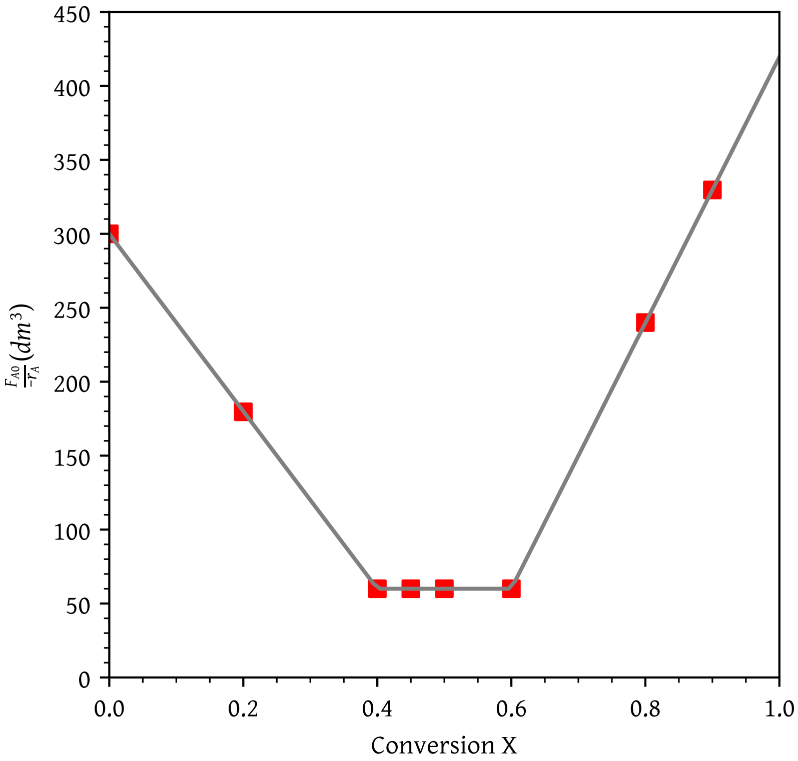

Figure 14: Piecewise linear fit processed data for problem 2-4

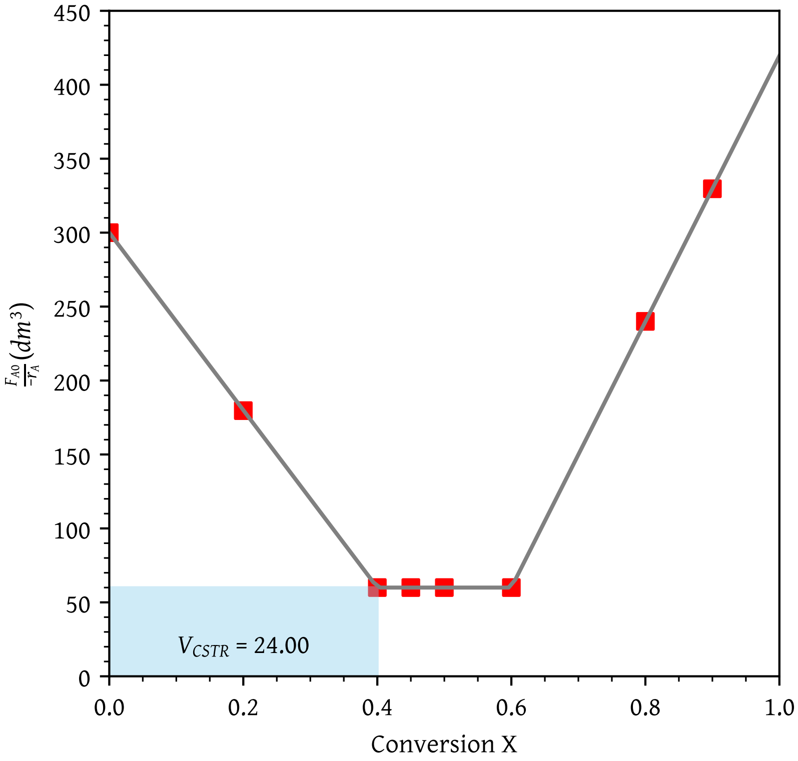

Figure 15: Reactor volume for CSTR to achieve X = 0.4

As the slope of $F_{A0}/-r_A vs. X$ line is 0 between 0.4 and 0.6, the CSTR and PFR volumes over this range would be identical.

(c) What is the maximum conversion that can be achieved in a $105 dm^3$ CSTR?

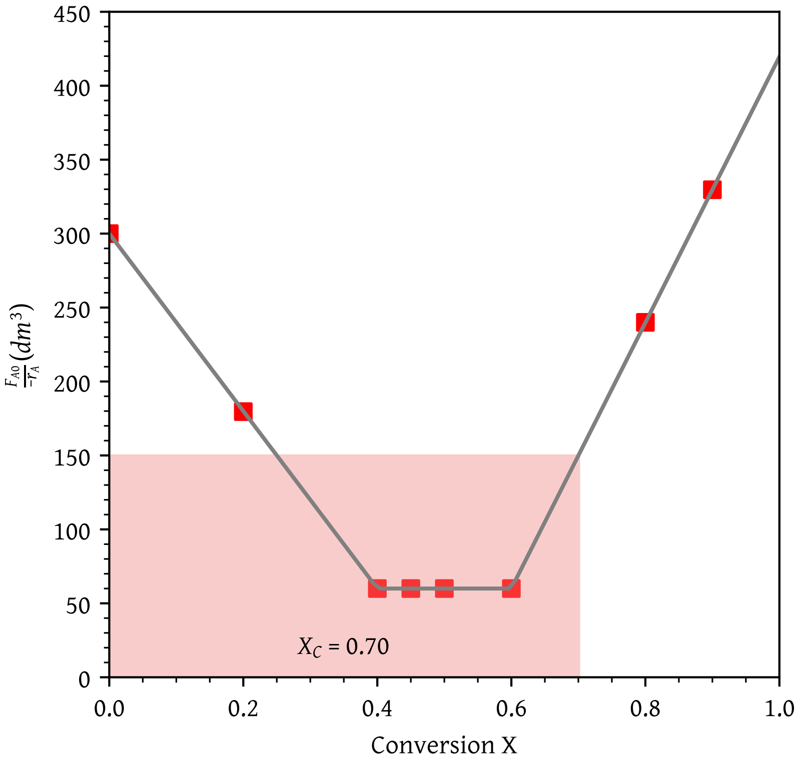

Figure 16: Reactor conversion for CSTR with volume = 105 dm^3

From Figure 16, X = 0.70.

(d) What conversion can be achieved if a $72dm^3$ PFR is followed in series by a $24dm^3$ CSTR?

From Figure 17, X_{PFR} = 0.40 and X_{CSTR} = 0.64.

(e) What conversion can be achieved if a $24dm^3$ CSTR is followed in a series by a $72dm^3$ PFR?

From Figure 18, X_{CSTR} = 0.40 and X_{PFR} = 0.91.

(f) Plot the conversion and rate of reaction as a function of PFR reactor volume up to a volume of $100dm^3$.

To create this plot (Figure 19), we will need to calculate the volume first for all X as

$$V = \int_0^x \frac{F_{A0} - r_A}{d} X$$

This data is given in Table 3

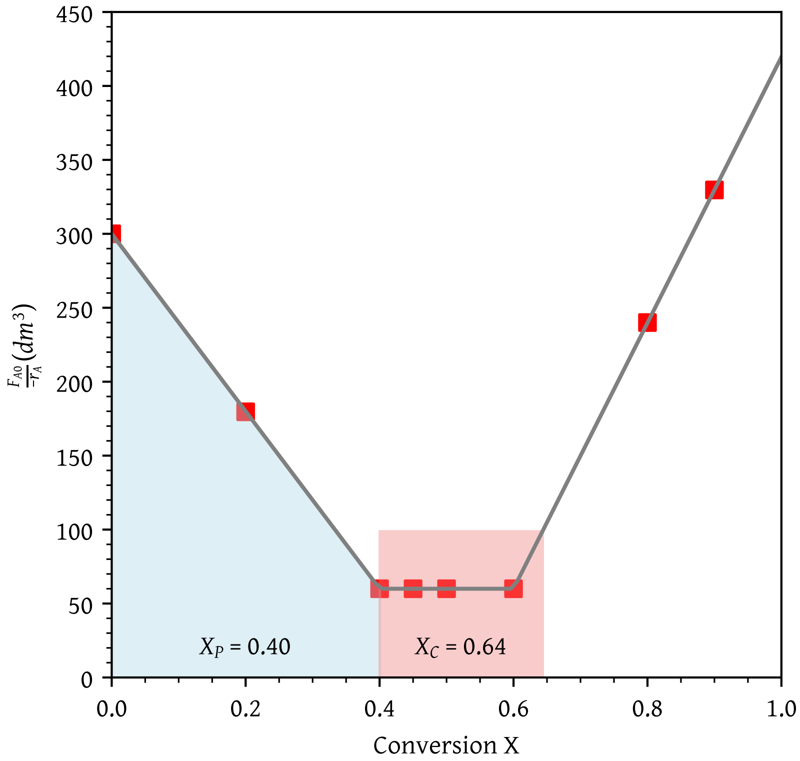

Figure 17: Reactor conversion for PFR followed by CSTR

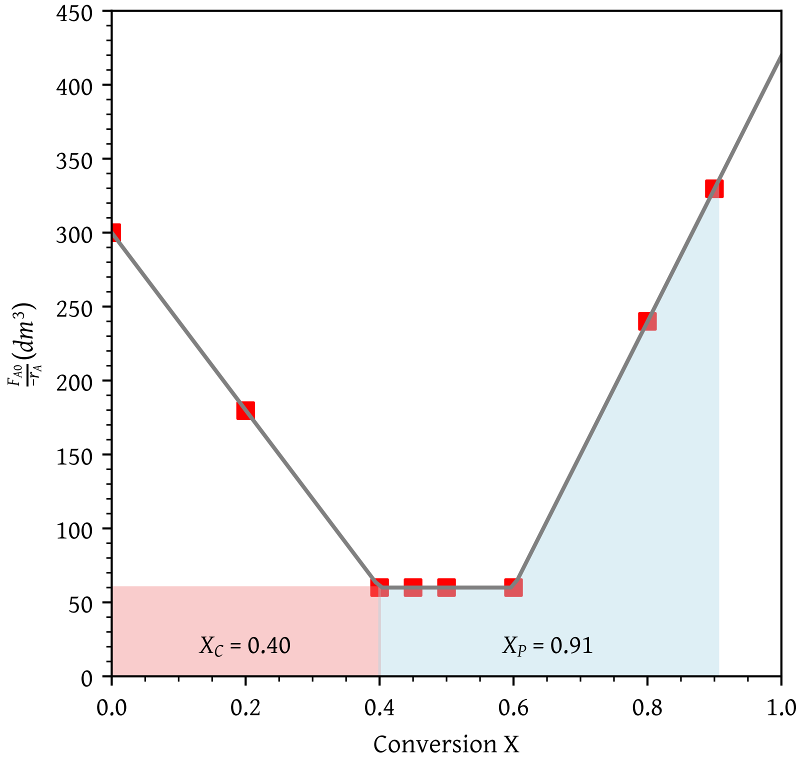

Figure 18: Reactor conversion for CSTR followed by PFR

Table 3: Reactor conversion and rate as function fo volume

$V(dm^3)$	X	$-r_A$
0	0	1
48	0.2	1.67
72	0.4	5
75	0.45	5
78	0.5	5
84	0.6	5
113.978	0.8	1.25
142.451	0.9	0.91

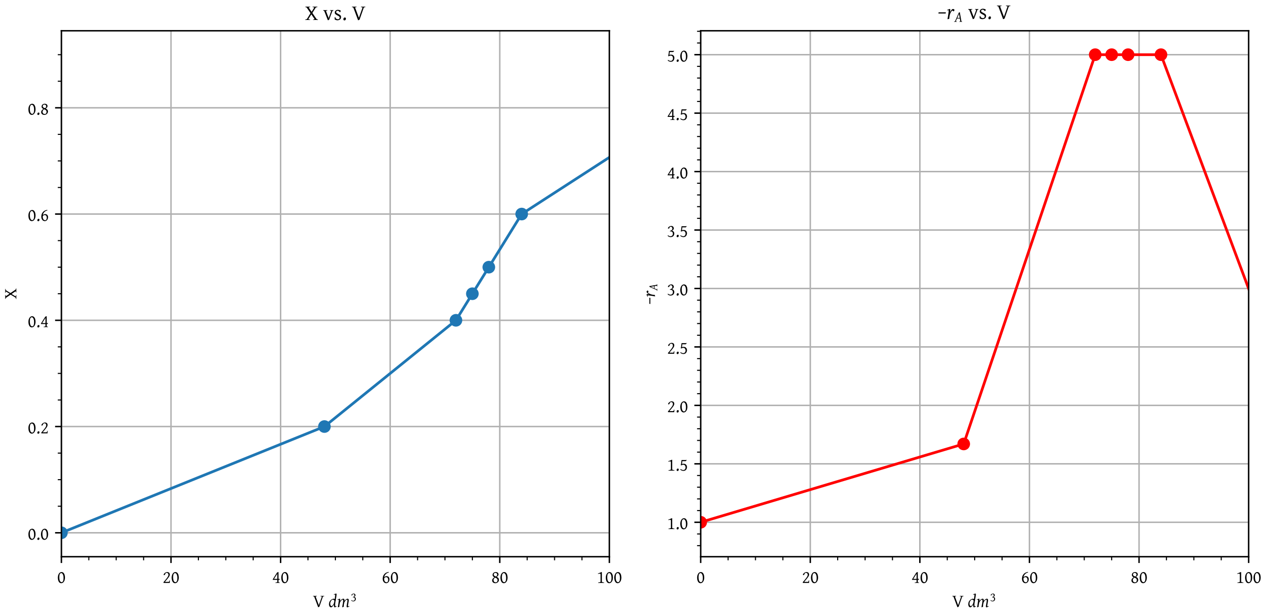

Figure 19: Reactor conversion and rate as function fo volume

Problem 3

P2-7: The adiabatic exothermic irreversible gas-phase reaction

$$2\,\mathrm{A} + \mathrm{B} \longrightarrow 2\,\mathrm{C}$$

is to be carried out in a flow reactor for an equimolar feed of A and B. A Levenspiel plot for this reaction is shown in Figure 20 .

(a) What PFR volume is necessary to achieve 50% conversion?
(b) What CSTR volume is necessary to achieve 50% conversion?
(c) What is the volume of a second CSTR added in series to the first CSTR (Part b) necessary to achieve an overall conversion of 80%?
(d) What PFR volume must be added to the first CSTR (Part b) to raise the conversion to 80%?
(e) What conversion can be achieved in a $6 \times 10^4 m^3$ CSTR? In a $6 \times 10^4 m^3$ PFR?

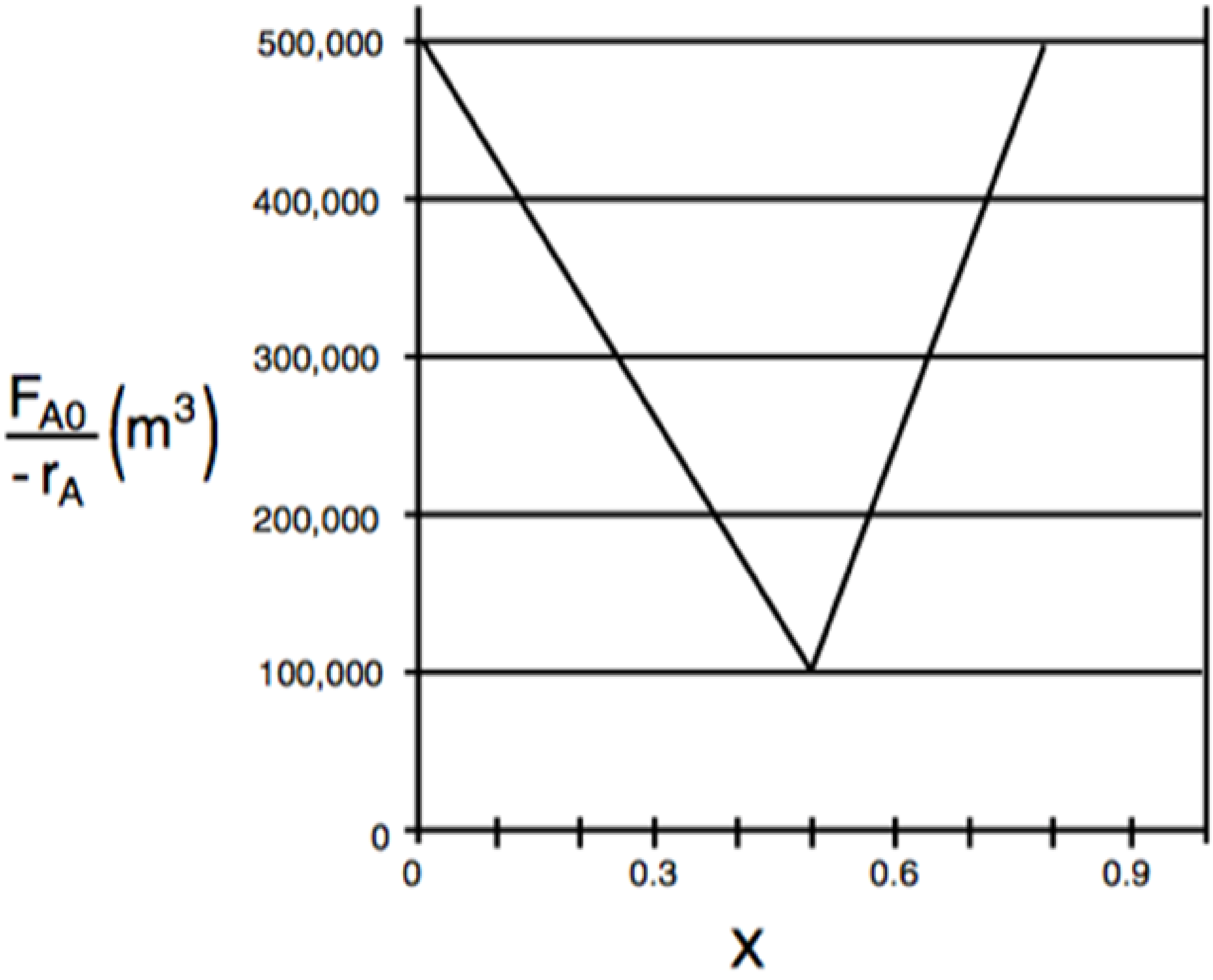

Figure P2-7$_B$ Levenspiel plot.

Figure 20: Figure-p2-7b

(f) Think critically to critique the answers (numbers) to this problem.

Solution:

Problem 4

P2.10: The curve shown in Figure 21 is typical of a gas-solid catalytic exothermic reaction carried out adiabatically.

(a) Assuming that you have a fluidized CSTR and a PBR containing equal weights of catalyst, how should they be arranged for this adiabatic reaction? Use the smallest amount of catalyst weight to achieve 80% conversion of A.
(b) What is the catalyst weight necessary to achieve 80% conversion in a fluidized CSTR?
(c) What fluidized CSTR weight is necessary to achieve 40% conversion?
(d) What PBR weight is necessary to achieve 80% conversion?
(e) What PBR weight is necessary to achieve 40% conversion?
(f) Plot the rate of reaction and conversion as a function of PBR catalyst weight, W.

Additional information: FA0 = 2 mol/s.

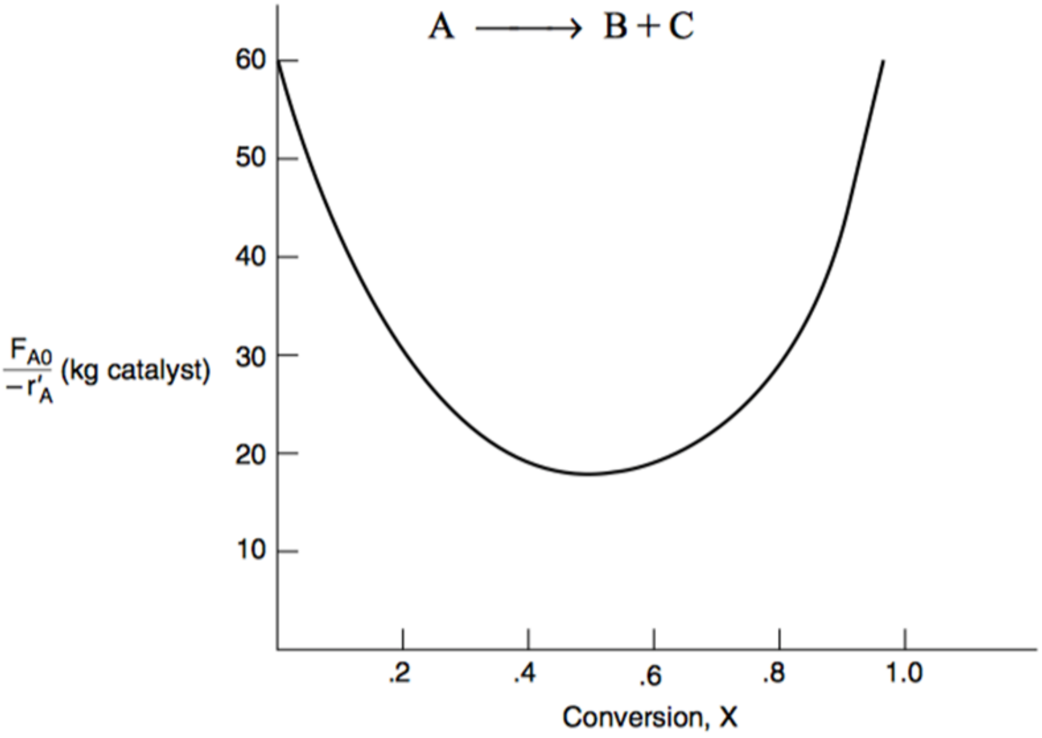

Figure P2-10$_B$ Levenspiel plot for an adiabatic exothermic heterogeneous reaction.

Figure 21: Figure P2-10b

Solution:

Digitized graph: (Figure 22)

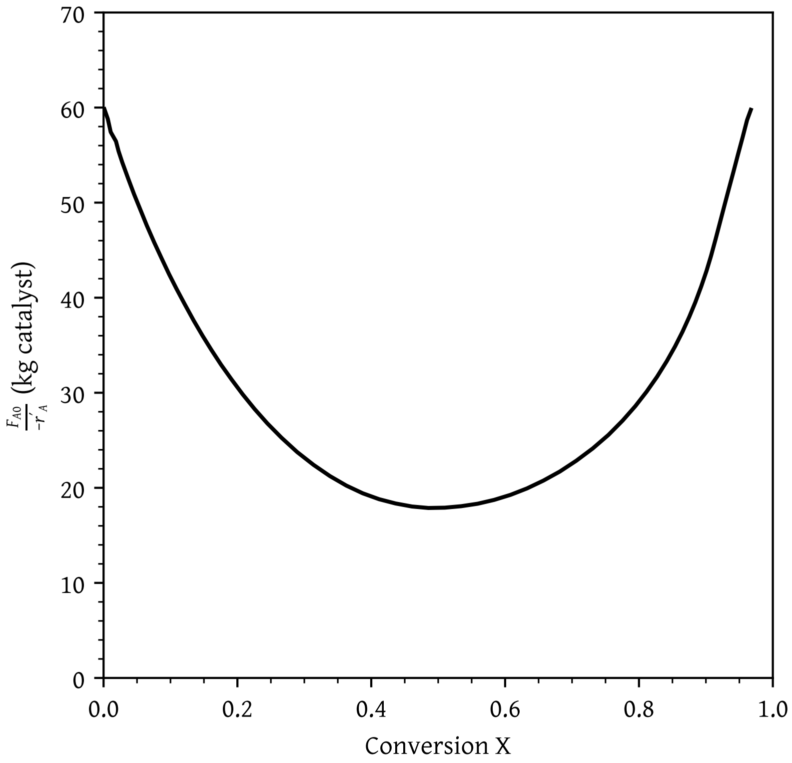

Figure 22: Levenspiel plot for an adiabatic exothermic heterogeneous reaction.

(a) Assuming that you have a fluidized CSTR and a PBR containing equal weights of catalyst, how should they be arranged for this adiabatic reaction? Use the smallest amount of catalyst weight to achieve 80% conversion of A. (Figure 23)

(b) What is the catalyst weight necessary to achieve 80% conversion in a fluidized CSTR? (Figure 24)

(c) What fluidized CSTR weight is necessary to achieve 40% conversion? (Figure 25)

(d) What PBR weight is necessary to achieve 80% conversion? (Figure 26)

(e) What PBR weight is necessary to achieve 40% conversion? (Figure 27)

(f) Plot the rate of reaction and conversion as a function of PBR catalyst weight, W. (Data table: Table 4; Plots: Figure 28)

Table 4: Reactor conversion and rate as function fo volume

$V(dm^3)$	X	$-r_A$
0.0730885	0.00122266	0.0334255
1.597	0.02795	0.0368764
3.97751	0.0756876	0.0436557
6.4248	0.134583	0.0531844
8.88462	0.207988	0.0670574
11.6107	0.313744	0.089225
14.0622	0.436315	0.108972
16.2747	0.55899	0.109126

Table 4: Reactor conversion and rate as function fo volume

$V(dm^3)$	X	$-r_A$
18.6969	0.681754	0.0921045
21.4901	0.794571	0.0699448
23.7561	0.865033	0.0549146
25.4624	0.907618	0.0450597
27.1073	0.941305	0.037535

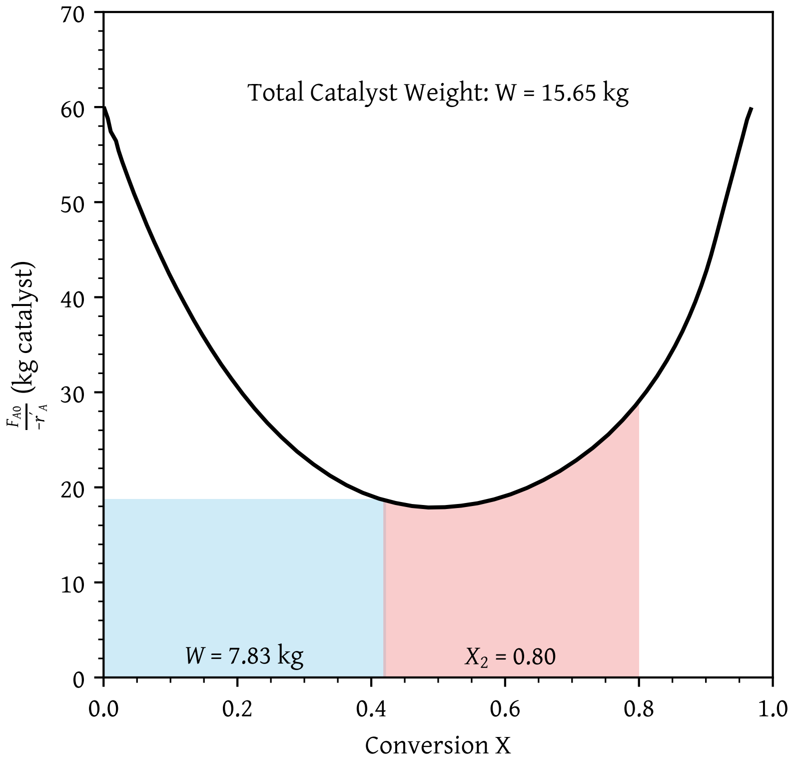

Figure 23: Levenspiel plot for an adiabatic exothermic heterogeneous reaction.

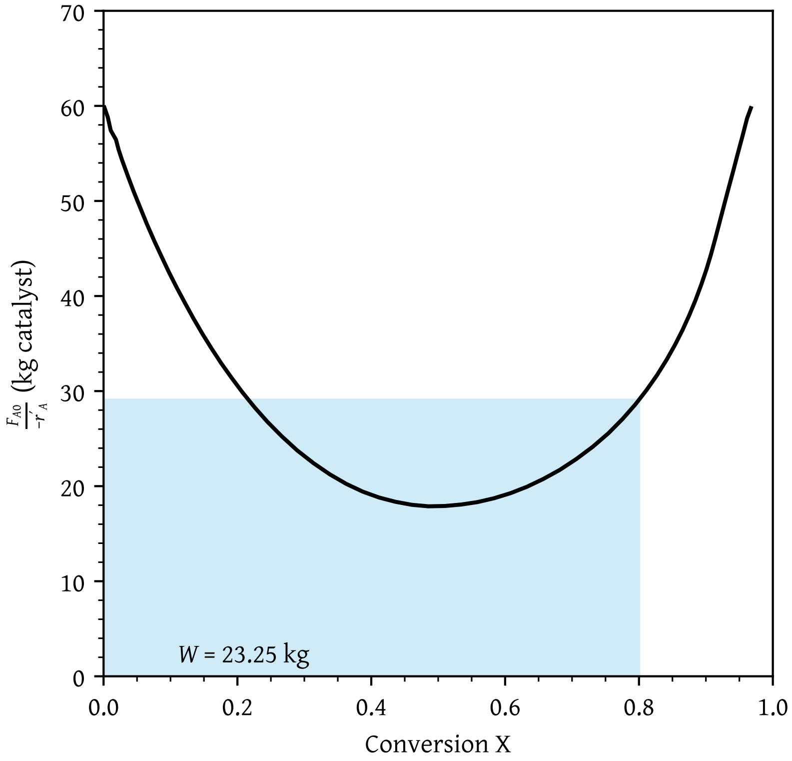

Figure 24: Catalyst weight for 80% conversion in CSTR

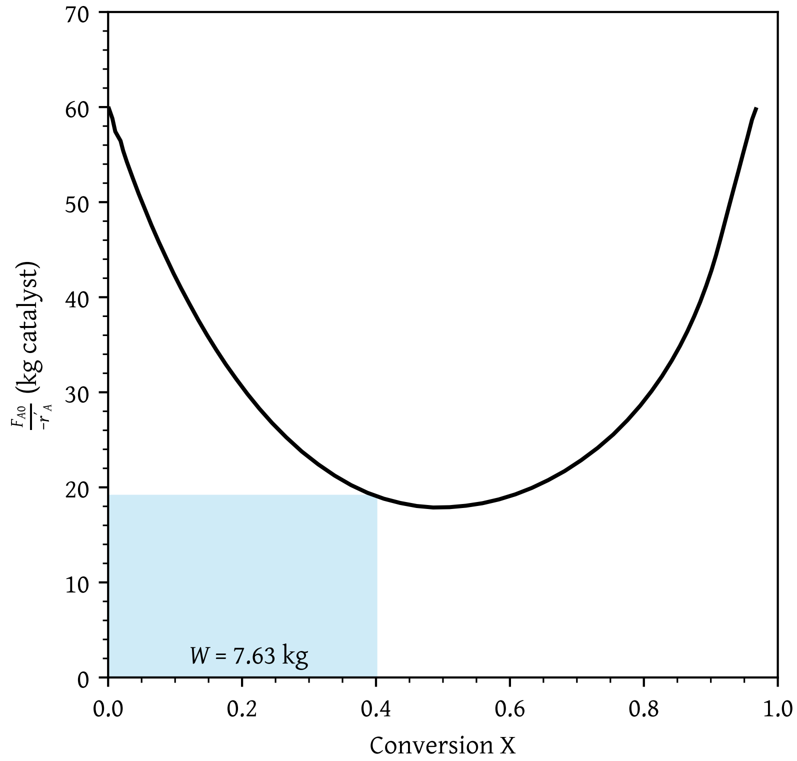

Figure 25: Catalyst weight for 40% conversion in CSTR

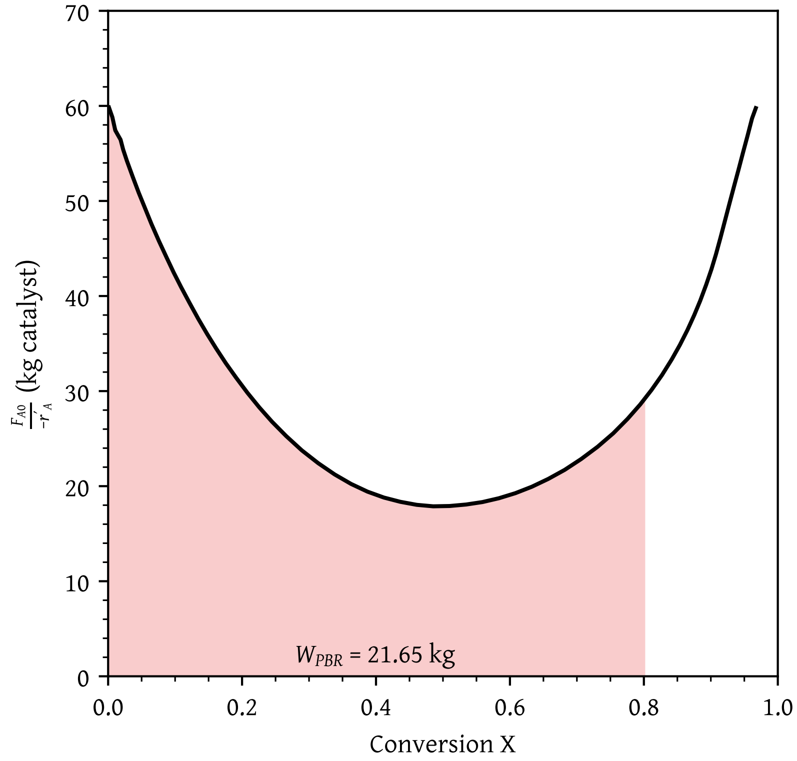

Figure 26: Catalyst weight for 80% conversion in PBR

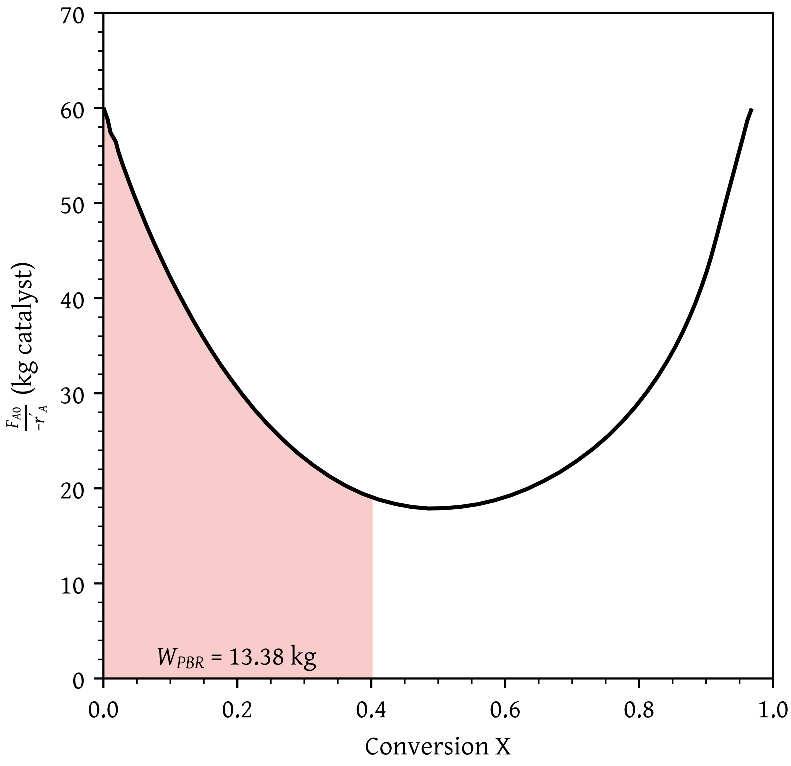

Figure 27: Catalyst weight for 40% conversion in PBR

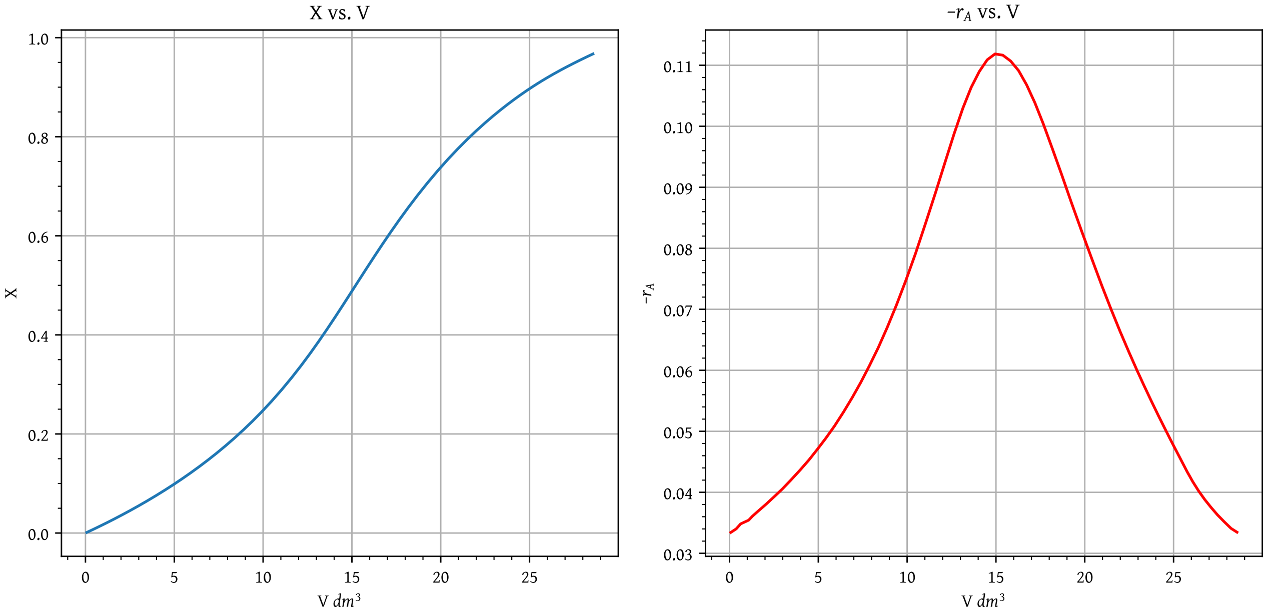

Figure 28: Reactor conversion and rate as function fo volume