

# Portfolio 04: Analysis of rate data

CHEN3010/ CHEN5040: chemical reaction engineering

**Student ID:**

## General Instructions for in class Portfolios

1. The portfolio is an open-book task.
2. You can use textbooks, the resources provided during class/ workshop etc. to answer the questions.
3. The portfolio task is made available in both pdf format and as a print.
4. You are free to choose a solution technique. It is **not** required that you use the provided python code to answer the questions. You can use any tool (pen and paper, excel, ... ) and any technique (graphical, numerical, analytical) that you are comfortable with.
5. Irrespective of your solution method, you are expected to write your answers on to the printed question paper provided. **This is what gets marked.**
6. The portfolio will take place during designated time slot communicated earlier by the unit coordinator. Please refer to the portfolio schedule on blackboard for the portfolio dates and topics.
7. The tasks will be a mix of theory questions, short calculation type and long numerical examples.
8. You have **30 minutes** to complete the tasks in the portfolio.
9. The portfolios will be marked immediately after completion by your peers using a provided marking rubric.
10. The portfolios will be collected by the instructors to verify peer marking and record the marks. You will receive your portfolio back within a week.
11. When you are required to upload the portfolio answers on to blackboard:
  - Save your report as a pdf file.
  - Rename the file as STUDENTID\_Portfolio\_x.pdf (Where STUDENTID is your student ID, and x is the portfolio number) and
  - Upload it using assessment submission link on blackboard.

## Academic Integrity

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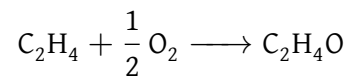
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# Introduction

Direct vapor phase oxidation of ethylene



was carried out in the presence of a silver catalyst in a differential reactor at 300 °C. Experiments were conducted at different partial pressures of  $\text{C}_2\text{H}_4$  and  $\text{O}_2$  and the effluent concentration of EO was measured. The measured rate data is shown in Table 1. (The data is available in csv format: [portfolio-4-raw-data.csv](#)).

Table 1: Raw data

Experiment	$P_{\text{C}_2\text{H}_4}$ (atm)	$P_{\text{O}_2}$ (atm)	$C_{\text{C}_2\text{H}_4\text{O}}$ ( $\text{mol}/\text{dm}^3 \times 10^4$ )
1	0.5	9.5	1.618
2	0.7	9.5	1.853
3	0.9	9.5	2.040
4	1.1	9.5	2.198
5	1.4	9.5	2.337
6	19.0	0.94	1.194
7	19.0	1.88	1.895
8	19.0	2.88	2.484
9	19.0	3.78	3.010
10	19.0	4.68	3.493

The exit volumetric flow rate from a differential packed bed containing 20g of catalyst was maintained at  $300 \text{ dm}^3/\text{min}$  for each run. The partial pressures of  $\text{C}_2\text{H}_4$  and  $\text{O}_2$  were determined at the entrance to the reactor, and the  $\text{C}_2\text{H}_4\text{O}$  concentration was measured at the reactor exit.

## Questions

1. Why do you think a differential reactor was used for these experiments? (2 marks)

2. In a step wise manner, outline the strategy (including any equations) you will use to analyze the data and determine the dependence of rate law on  $P_{\text{C}_2\text{H}_4}$  and,  $P_{\text{O}_2}$ . (14 marks)

3. Based on the data calculate the rates of reaction.

(4 marks)

4. Determine the rate law and rate law parameters. Report your values of the orders of reaction with respect to  $P_{\text{C}_2\text{H}_4}$  and,  $P_{\text{O}_2}$  and reaction rate constant  $k$  (in  $\text{mol}/\text{atm kg} - \text{cat s}$ ). Skeleton python code is provided at the end of the portfolio statement. Report all relevant statistical data (such as slope, intercept, and  $R^2$  value for a linear fit; error estimates (optimality) for least squares fit) (8 marks)

5. What is the limitation of current experimental program in context of deriving the rate law?  
How will you overcome it? (2 marks)



## Skeleton code

```
import numpy as np
from scipy.stats import linregress
from scipy.optimize import least_squares
import matplotlib.pyplot as plt

Temperature = 300 # deg. C
DeltaW = 20 # g
V_0 = 300 # dm3/min

# Define the data type for each field
dtype = [
    ('Run', int),          # Run number (experiment number)
    ('P_c2h4', float),    # Pressure of C2H4 in atm
    ('P_o2', float),      # Pressure of O2 in atm
    ('C_c2h4o', float)    # Concentration of C2H4O in mol/dm3 x 104
]

# Data for each experiment
data = np.array([
    (1, 0.5, 9.5, 1.618),
    (2, 0.7, 9.5, 1.853),
    (3, 0.9, 9.5, 2.040),
    (4, 1.1, 9.5, 2.198),
    (5, 1.4, 9.5, 2.337),
    (6, 19.0, 0.94, 1.194),
    (7, 19.0, 1.88, 1.895),
    (8, 19.0, 2.88, 2.484),
    (9, 19.0, 3.78, 3.010),
    (10, 19.0, 4.68, 3.493)
], dtype=dtype)

pc2h4 = data["P_c2h4"]
po2 = data["P_o2"]
cc2h4o = data["C_c2h4o"]*1e-4

# Calculate rate

# Select appropriate data for analysis

# Example code
# first data point has index 0
# x_a = x[1:n] # Selects data points 2 to n from x array

# transform the data for analysis

# example code for linear regression
# log_x = np.log(x) # calculate log
```

```

# res = linregress(x,y) # fit line
# slope, intercept, and r value can be accessed using res.slope,
# res.intercept, res.rvalue
# line = res.slope * x + res.intercept # Create a line from linear regression

# Print results
# print (res.slope, res.intercept, res.rvalue)

# example code for least_squares
# Objective function to minimize: the difference between rate (experimental)
# and rate (calculated)
#def objective(params, *args):
#    a, b = params
#    x, y_obs = args
#
#    # calculate objective function
#    y_calc = (a * x**b) # Replace with your own expressions
#    return y_obs - y_calc
#
# # Initial guesses
# a = 1
# b = 1
#
# guess = np.array([a,b])
# bounds = (
#     [1e-3, 1e-3], # lower bound
#     [1e3, 1e3]    # upper bound
# )
# args = (x,y_obs)
#
# # Minimize the objective function
# result = least_squares(objective, guess, args=args, bounds=bounds)
#
# # Extract the results
# a_fit, b_fit = result.x
# optimality = res.optimality
#
# Print results
# print (a_fit, b_fit)

# Plotting

# Example code

# plt.plot(x,y, label="y") # Normal plot
# plt.loglog(x, y, 'o', label='Experimental') # log - log plot scatter points
# plt.show()

```