NATIONAL UNIVERSITY OF SCIENCE AND TECHNOLOGY

FACULTY OF INDUSTRIAL TECHNOLOGY

DEPARTMENT OF CHEMICAL ENGINEERING

Computational Methods for Chemical Engineers

ECE1205

Final Examination Paper

October 2024

This examination paper consists of 5 pages

Time Allowed: 3 hours

Total Marks: 100

INSTRUCTIONS

1. Answer **Section A** and any other **three (3)** questions
2. Each question carries 25 marks
3. The use of calculators is permissible

MARK ALLOCATION

QUESTION	MARKS
1A	25
1B	25
2B	25
3B	25
4B	25
TOTAL ATTAINABLE	100

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SECTION A
Answer this question

QUESTION A1

a) What are Boolean operators? Give 5 examples. **[5]**

b) Give steps for drawing a scatter graph in Excel. **[4]**

c) There are a number of default functions in excel state any four. **[4]**

d) State the functions of these modules in Python i) Matplotlib, ii) SciPy and iii) NumPy **[6]**

e) Three regions are marked in Spyder interface (1-3). State their names and functions.
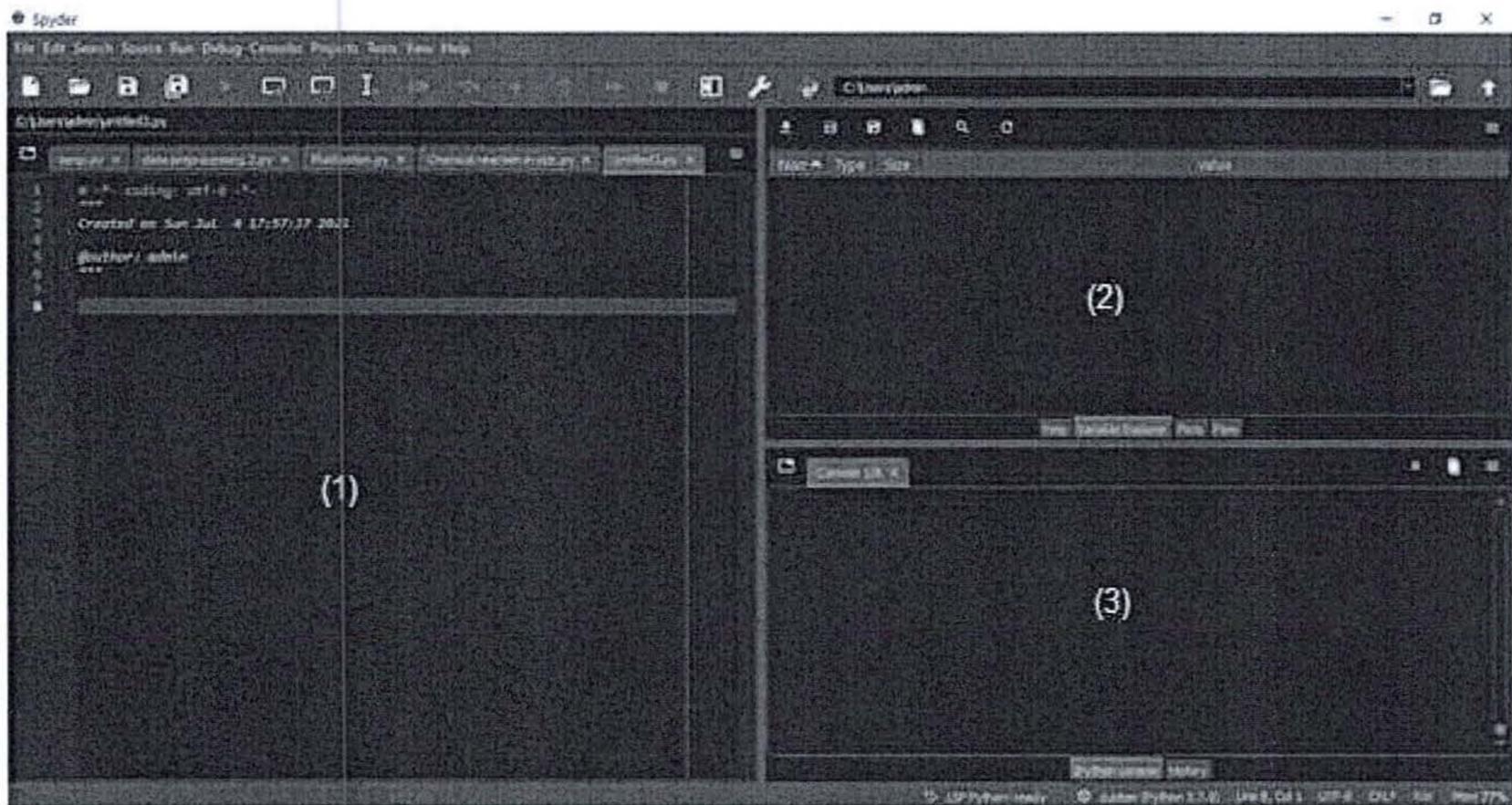
[6]

QUESTION B1

Excel is a versatile software that can be used for a number of tasks. With an appropriate spreadsheet and supporting text explain how you would solve the following problems:
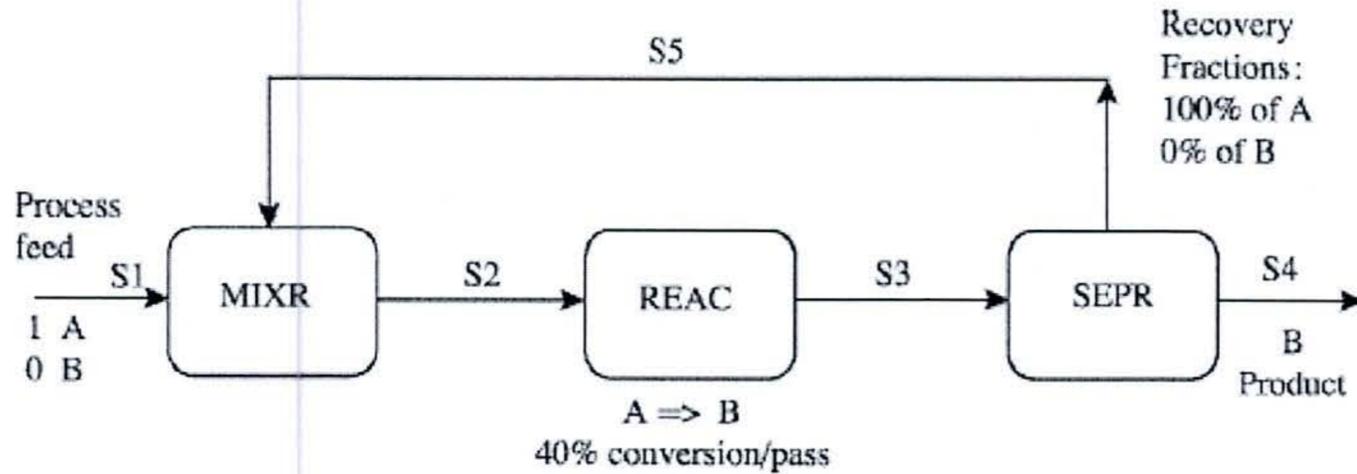
a) The equation given below using solver.

$$x^2 - 2x = 1$$
[5]

b) The material balance for the system described below:

Consider a simple process in which the reactor can only convert 40 percent of the feed to it (perhaps due to equilibrium constraints), but the separation of reactant A and product B is complete and the unreacted A is recycled.

i) Describe how would you do this material balance on excel (based on A molecule). **[6]**

ii) Do the actual calculation using iteration to determine the streams at steady state (based on A

molecule). **[6]**

c) There are four collection data types in the Python programming language. State them and state their properties. **[8]**

QUESTION B2

a) Discuss what is Python? Give three applications. **[5]**

b) Write a script to the numerical solution to the following differential equation with its associated initial conditions: $y(0) = 5$.

$$\frac{dy(t)}{dt} = -0.3y(t)$$

[12]

c) Write a Python program that calculates the volume of a rectangular prism. The program should prompt the user to input the length, width, and height of the prism. Then, it should compute and display the volume using the formula:

Volume=Length×Width×Height

[8]

QUESTION B3

a) The script below is for a simple ordinary differential equation. Solve this differential and draw the graph as represented by the code below.

```
8     from scipy.integrate import odeint
9     import matplotlib.pyplot as plt
10    import numpy as np
11    def f(y, t):
12    # this is the rhs of the ODE to integrate , i.e. dy/dt=f(y,t)
13        return 1/2
14    y0 = 1 # initial value
15    a = 0 # integration limits for t
16    b = 1
17    tspan = np. arange (a, b, 0.05) # values of t for which we require the solution y(t)
18    y = odeint (f, y0 , tspan) # actual computation of y(t)
19    # plot the solution
20    plt . plot (tspan, y)
21    plt . xlabel ('t'); plt . ylabel ('y(t)')
22    plt . show ()
23    # print the solution
24    print(tspan, y)
```

[12]

b) Perform a mass balance for the system given below. Ammonia is produced via the Haber-Boch process in which nitrogen is extracted from the atmosphere and reacted with hydrogen in the following reaction.

$$N_2 + 3H_2 \leftrightarrow 2NH_3 \qquad \Delta H_r^o = -45.8 \, kJ/mol$$

In a simplified process, a feed stream containing 200 mol/h of N_2 and 600 mol/h of H_2 is mixed in a reactor where equilibrium conversion of N_2 is 25 mol%. The reaction products are sent to a separator where 98% of the ammonia and 0.5% each of N_2 and H_2 is recovered in the product stream. [13]
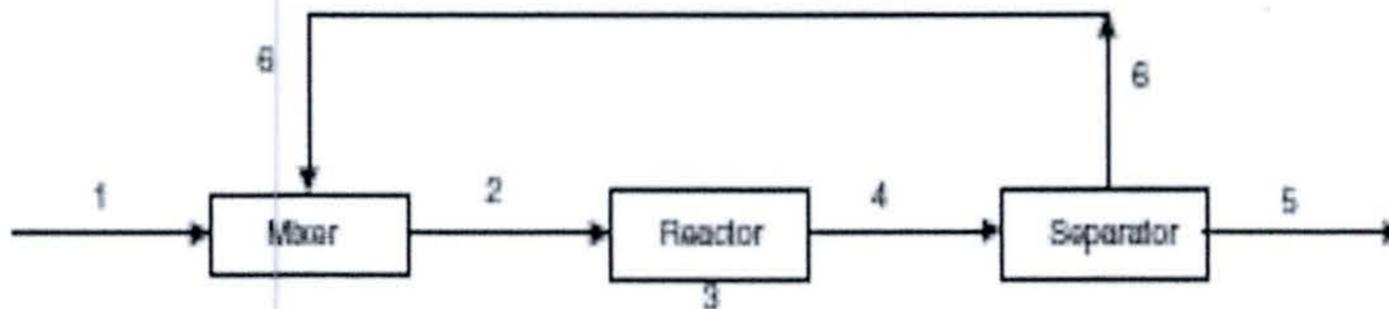
QUESTION B4

a) Write a script to the numerical solution to the following differential equation with its associated initial conditions.

$$\frac{dy(t)}{dt} = -y(t) + 1$$

[10]

b) A python code is given to calculate the pressure drop of a pipe than is 100 m. The user can input a desired flow rate (m³/s).

i) The user upon attempting to run this code they got this syntax error

```
Traceback (most recent call last):

  File "C:\Users\admin\exam friction lossessss.py", line 17, in <module>
    v = 4*Q/(np.pi*d**2)

TypeError: unsupported operand type(s) for /: 'str' and 'float'
```

debug the code for the user and highlight what was the source of error.   [5]

ii) Perform the task outlined by this code and give the outputs. The input value for volumetric flow rate is 0.0000032 m³/s (3.2 litres/s).   [10]

```python
import numpy as np

Q = input()# 0.0000032 Flow rate m^3/s
d = 0.002  # Pipe's diameter m
mu = 0.001                # Water viscosity Pa s @25 C
rho = 1000                # Water density kg/m^3
L = 100                    # Pipe's length m
e = 0.00005                # Pipe's rugosity
# This function calculates the velocity of the fluid

v = 4*Q/(np.pi*d**2)
print('velociy (m/s): ' + str(v))
# This function calculates the friction coefficient Lambda

reynolds = rho*v*d/mu
print('reynolds:' + str(reynolds))
    # If RE < 3000 flow is laminar, otherwise it is turbolent
if reynolds <= 3000:
        lbda = 64/reynolds
else:
        lbda = 0.3164/reynolds**2

print('friction factor: ' + str(lbda))


# This function calculates the pressure drop
pDrop = 4 * lbda * v**2 *rho*  L/ d

print('pDrop:   ' + str(pDrop))
```