ChEn-3170: Computational Methods in Chemical Engineering Fall 2018 UMass Lowell; Prof. V. F. de Almeida **20Dec2018**

Final Exam 20Dec2018 Session 801/802

Name:

Guidance:

- This is a closed-book, closed-note, individual exam.
- You may use an off-line, simple calculator, that does not store documents or notes.
- You may use scratch paper if you wish (paper will be provided).
- All pages must be submitted with your completed exam.
- Make sure to answer the question asked.
- Show your work and be clear.

Rubric Panel

Show No.	Now Showing (3 - 6)	Value	Score
1-5	Jupythonic Park	50	
6	Relax...Relax...	20	
7	Just One More Time	20	
8	Fast and furious	10	
	Total	100	

Show Problem 1 (10 pts)

Name and give an example of the four main data structures in Python used in this course. Write your example as you would do in a Jupyter program cell below and initialize each of the data structures as empty.

In [ ]:
```
'''1.1 Data structure'''
```

In [ ]:
```
'''1.2 Data structure'''
```

In [ ]:
```
'''1.3 Data type'''
```

In [ ]:
```
'''1.4 Data type'''
```

Show Problem 2 (10 pts)

In each of the cells below compute the result as it would show if the cell were executed by the Python interpreter.

In [ ]:
```
'''2.1 (4pts)'''

vec_a = (2,1,0)
vec_b = (8,6,7)
vec_c = vec_a + vec_b
print(vec_c)
print(len(vec_c))
```

In [ ]:
```
'''2.2 (4pts)'''

row_1 = [2,1,6]
row_2 = [0,-1,5]
row_3 = row_1 + row_2
print(row_3)
print(len(row_3))
```

In [ ]:
```python
'''2.3 (2pts)'''

text = 'compute the result'
print(len(text))
```

Show Problem 3 (10 pts)

3.1 (2pts) Given matrices $\mathbf{A}$ and $\mathbf{B}$ compute $\mathbf{C} = \mathbf{A}\,\mathbf{B}$. Write the simplest Python code you can imagine to performe this operation and compute and print the result. Note: $\mathbf{A} = \begin{pmatrix} 1 & 2 & -4 \\ 0 & 3 & 4 \\ 1 & 2 & 5 \end{pmatrix}$ and $\mathbf{B} = \begin{pmatrix} 1 & 7 & 3 \\ 3 & 2 & 6 \\ 0 & 2 & 4 \end{pmatrix}$.

In [ ]:
```
'''3.1 (2pts) Code and result'''
```

3.2 (4pts) Given matrix $\mathbf{A}$ and vector $\mathbf{b}$ compute the solution $\mathbf{x}$ of $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ and write the simplest possible Python code to compute and print the result. Note: $\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ -1/2 & 1 & 1 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$.

In [ ]:
```
'''3.2 (4pts) Code and result'''
```

3.3 (4pts) Given matrix $\mathbf{A}$ and vector $\mathbf{b}$ compute the solution $\mathbf{x}$ of $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ and write the simplest possible Python code to compute and print the result. Note: $\mathbf{A} = \begin{pmatrix} 2 & 3 & 1 \\ 0 & 1/2 & 1/2 \\ 0 & 0 & 1 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 1 \\ 5/2 \\ 0 \end{pmatrix}$.

In [ ]:
```
'''3.3 (4pts) Code and result'''
```

Show Problem 4 (10 pts)

a) (5pts) Given matrix $\mathbf{A}$ compute the solution $\mathbf{A}\,\mathbf{x} = \mathbf{b}$. Write the simplest Python code you can imagine to performe this operation and compute and print the result. Note:
$\mathbf{A} = \begin{pmatrix} 2 & 3 & 1 \\ 1 & 2 & 1 \\ -1 & -1 & 1 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$.

In [ ]:
```
'''4.1 Solve A x = b'''
```

b) (5pts) Given matrix **A** compute the solution $\mathbf{A}\,\mathbf{x} = \mathbf{b}$. Write the simplest Python code you can imagine to performe this operation and compute and print the result. Note:

$$\mathbf{A} = \begin{pmatrix} 2 & 3 & 1 \\ 1 & 2 & 1 \\ -1 & -1 & 0 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}.$$

In [ ]:
```
'''4.2 Solve A x = b'''
```

Show Problem 5 (10 pts)

Given the following reaction mechanism for hydrogen bromide:

$$\begin{aligned} H_2 + Br_2 &\longleftrightarrow 2\,HBr \\ Br_2 &\longleftrightarrow 2\,Br \\ Br + H_2 &\longleftrightarrow HBr + H \\ H + Br_2 &\longleftrightarrow HBr + Br \\ H + HBr &\longleftrightarrow H_2 + Br \\ 2\,Br &\longleftrightarrow Br_2 \end{aligned}$$

write a simple code to compute the number of independent reactions and compute this number.

In [ ]:
```
'''5. Independent reactions'''
```

Show Problem 6 (20 pts)

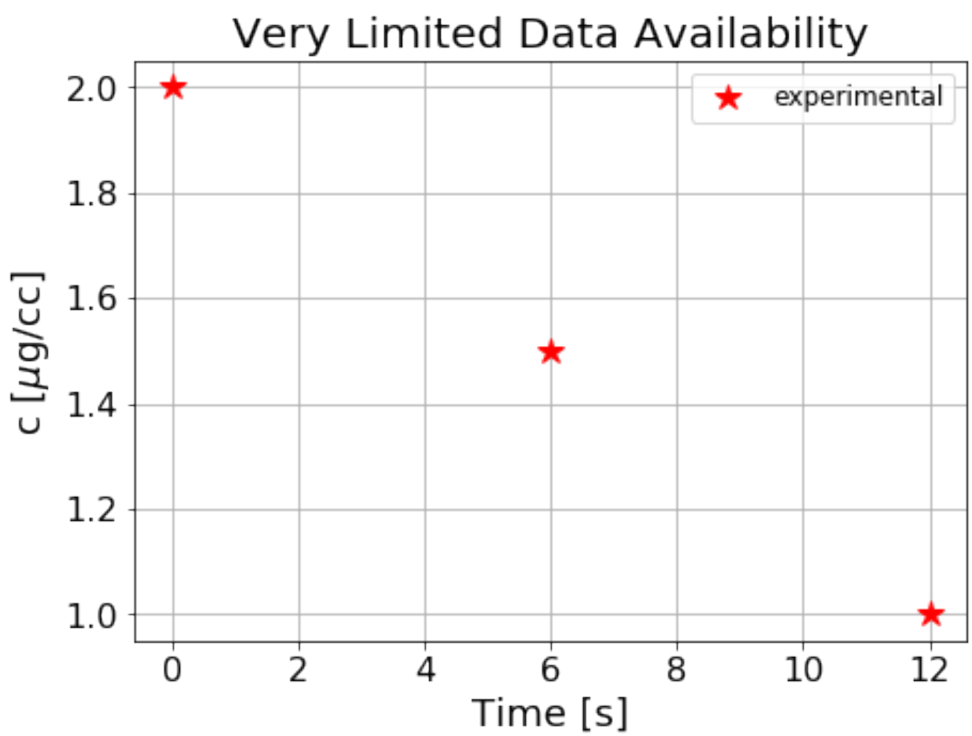
A concentration signal is believed to follow the model

$$c(t) = a + b\, e^{-t/\tau_1} + c\, e^{-t/\tau_2}$$

which has two modes of relaxation with relaxation times, $\tau_1 = 2$ s, and $\tau_2 = 4$ s. Given the scarce measurements of $c(t)$ below:

1. Calculate the best values of a, b, c that fit the model.
2. Calculate the residual of your best approximation.
3. Is this a good approximation for the data? (hint: calculate $c(1)$ and/or graph the approximant $c(t)$ on the plot)
4. Explain why or why not the approximation is good and the conditions that control the goodness of the approximation.

In [6]:
```
'''Data'''
```



In [ ]:
```
'''6.1 Calculate optimum a, b, c'''
```

In [ ]:
```
'''6.2 Calculate the residual'''
```

In [ ]:
```
'''6.3 Is this a good approximation of the data?'''
```

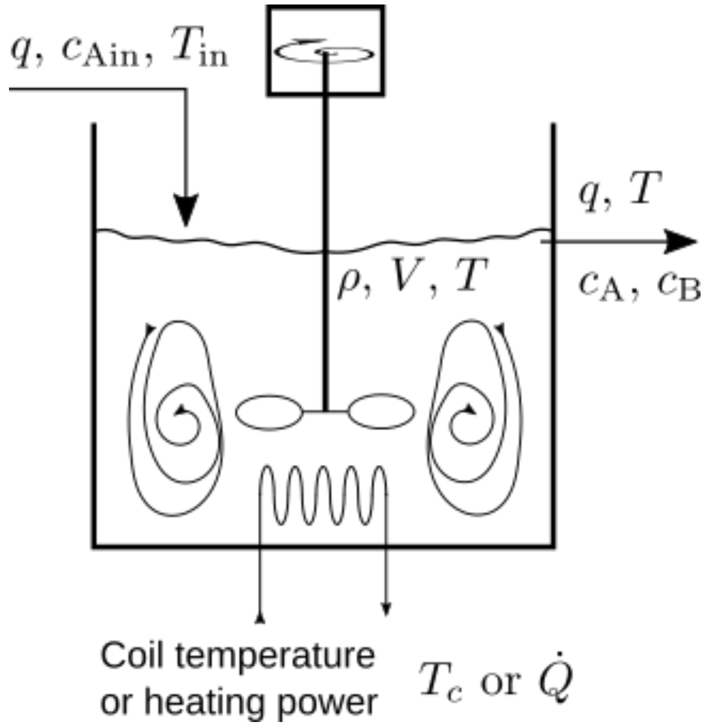
In [ ]:
```
'6.4 Explain why or why not the approximation is good and the conditions t
```

Show Problem 7 (20 pts)

A reversible first-order endothermic reaction

$$\mathrm{A} \underset{k_\mathrm{b}}{\overset{k_\mathrm{f}}{\rightleftarrows}} 2\,\mathrm{B},$$

is performed in a continuous-stirred-tank reactor.



The experimental forward rate of reaction per unit volume is

$$r_{\mathrm{f},1} = k_\mathrm{f}\, c_\mathrm{A}\, c_\mathrm{B}^0,$$

and the reverse is

$$r_{\mathrm{b},1} = \lambda\, k_\mathrm{f}\, c_\mathrm{A}^0\, c_\mathrm{B}^\beta.$$

The governing equations for the time variation of the concentrations of species A and B are:

$$\frac{dc_\mathrm{A}}{dt} = -\frac{1}{\tau}\left(c_\mathrm{A} - c_\mathrm{Ain}\right) + g_\mathrm{A}(t),$$
$$\frac{dc_\mathrm{B}}{dt} = -\frac{1}{\tau}\left(c_\mathrm{B} - c_\mathrm{Bin}\right) + g_\mathrm{B}(t),$$

where $\tau = \frac{V}{q} = \frac{V\rho}{w}$ is the residence time of the flow in the reactor tank, and $\mathbf{g} = \begin{pmatrix} g_\mathrm{A} \\ g_\mathrm{B} \end{pmatrix}$ is the species production vector obtained from the stoichiometric relation

$$\mathbf{S}^\top\, \mathbf{r} = \mathbf{g},$$

using $\mathbf{r} = r_{\mathrm{f},1} - r_{\mathrm{b},1}$.

The following values are given

Name	Parameter	Value	Unit
mass flow rate	w	10	kg/s

inflow concentration of A	c_{Ain}	1.2	kgmol/m^3
inflow concentration of B	c_{Bin}	0.0	kgmol/m^3
holdup volume	V	0.2	m^3
mass density	ρ	1000	kg/m^3
Arrhenius frequency	k_0	1.97×10^{24}	s^{-1}
activation temperature	E/R	20000	K
reverse reaction factor	λ	0.1	
reverse reaction order	β	2.5	
S.S. reactor temperature	T_{ss}	350	K

When the reactor reaches steady state (temperature $T_{\text{ss}} = 350$ K), the forward reaction constant k_{f} is given by the Arrhenius relation: $k_{\text{f}} = k_0 \, \exp(\frac{-E}{R\,T})$ at the steady state temperature. Compute the concentration of A and B at steady state.

In [ ]:
```python
'''7 Compute the steady state concentration of A and B'''
```

Show Problem 8 (10 pts)

If the flow rate through the tank in Problem 7 is too high, the species generation terms are negligible. In this limit, calculate:

1. The time-dependent behavior of the concentrations of A and B assuming that the starting concentrations in the tank are the values of the steady state computed in Problem 7.
2. What would be the temperature in the tank?

In [ ]:
```
'''8.1a (4pts) Solve for c_a(t)'''
```

In [ ]:
```
'''8.1b (4pts) Solve for c_b(t)'''
```

In [ ]:
```
'''8.2 (2pts) Temperature in the tank'''
```