ChE445_HW1_Winter2020

January 22, 2020

Q1. Ideal PFR: mean residence time and space time.

A gas-phase first-order reaction $A \rightarrow B + 2C$ is carried out isothermally in an ideal PFR of $533L$ volume with no pressure drop. The rate constant is $0.032 min^{-1}$, pure A enters the reactor, $C_{A0} = 0.5M$, $F_{A0} = 2 mol/min$. 80% conversion is achieved in the reactor. Find mean residence time and space time. Explain the difference if any.

Answer1.

Stoichiometric Table for $A \rightarrow B + 2C$

.	Initial	Final
A	F_{A0}	$F_{A0}(1-X)$
B	0	$F_{A0}X$
C	0	$2F_{A0}X$
Total	F_{A0}	$F_{A0}(1+2X)$

$\frac{Q}{Q0} = \frac{F_T}{F_{T0}} = 1 + 2X$

Space time: $\tau = \frac{V}{Q0} = \frac{V.C_{A0}}{F_{A0}}$

$-r_A = kC_A = k\frac{F_A}{Q} = k\frac{F_{A0}(1-X)}{Q_0(1+2X)} = kC_{A0}\frac{1-X}{1+2X}$

Mean residence time: $\bar{t} = \int_0^V \frac{dV}{Q} = F_{A0}\int_0^X \frac{dX}{-r_A.Q} = C_{A0}\int_0^X \frac{dX}{-r_A(1+\epsilon X)}$

$\bar{t} = C_{A0}\int_0^X \frac{(1+2X)dX}{kC_{A0}(1-X)(1+2X)} = \frac{1}{k}ln\frac{1}{1-X}$

[86]:
```
import numpy as np
import math

V=533
CA0=0.5
FA0=2
k=0.032
X=0.8

Tau=V*CA0/FA0
Tbar=(1/k)*(math.log (1/(1-X)) )

print('Space time          =', Tau, 'min')
print('mean residence time =', "{0:.3f}".format(Tbar), 'min')
print('---------------------------------')
```

```
print('mean residence time < Space time because fluid expands')
```

```
Space time           = 133.25 min
mean residence time = 50.295 min
---------------------------------
mean residence time < Space time because fluid expands
```

Q2. Ideal CSTR: mean residence time and space time.

A liquid-phase reaction $A + 2B \rightarrow C$ is carried out in a CSTR of $40L$ volume. The feed is stoichiometric, its volumetric flow rate $Q_0 = 200L/h$. 45% conversion is achieved. Find mean residence time and space time. Explain the difference if any.

Answer2. Space time: $\tau = \frac{V}{Q0}$

Mean residence time: $\bar{t} = \frac{V}{Q_{exit}}$

This reaction is happening in an incompressible fluid and it is assumed that the liquid phase does not have any density changes

$Q_{exit} = Q_0$ and $\bar{t} = \tau$

[87]:
```
V=40    #L
Q0=200  #L/h



Tau=V/Q0

print('Space time', Tau, 'h')
print('---------------------------------')
print('In an incompressible fluid:    Space time = Mean residence time ')
```

```
Space time 0.2 h
---------------------------------
In an incompressible fluid:    Space time = Mean residence time
```

Q3.(Review of ChE 345)

A packed-bed reactor is to be designed to achieve 80% conversion in a first-order constantdensity reaction. A research paper reports a PBR used for this reaction for the same feed composition and operating conditions except that 40% conversion was achieved with $1kg$ of catalyst. To double the conversion from the reported 40% to the required 80%, how much catalyst mass is required? Assume that it is an ideal PBR (ideal PBR mole balance is the same as ideal PFR mole balance, except that catalyst mass W is used instead of reactor volume V.)

Answer3.

MB in a PBR: $\frac{dF_A}{dW} = r_A$

Rate law: $r_A = kC_A$

Stoichiometry: $C_A = \frac{F_A}{Q}$ for a constant density case: $C_A = \frac{F_{A0}(1-X)}{Q_0}$

Therefore: $\frac{dF_A}{dW} = k\frac{F_{A0}(1-X)}{Q_0}$

$F_{A0}\frac{dX}{dW} = k\frac{F_{A0}}{Q_0}(1 - X)$

$ln(\frac{1}{1-X}) = \frac{k}{Q_0}W$

$\frac{k}{Q_0} = ln(\frac{1}{1-X})/W$

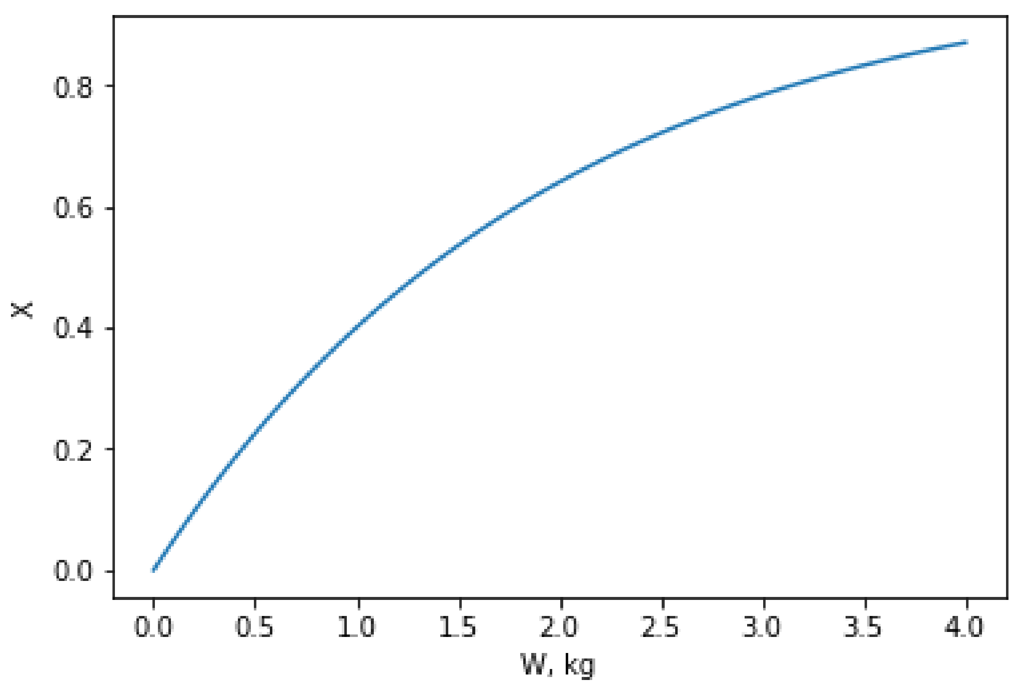
$X = 1 - 1/(e^{\frac{k}{Q_0}*W})$ Conversion does not increase linearly with W.

[91]:
```
import numpy as np
import math

W=1 #kg
X=0.4

KQ0=(math.log(1/(1-X)))/W

print('k/Q0=', "{0:.3f}".format(KQ0), '1/kg')
print('-----------------')
```

```
k/Q0= 0.511 1/kg
-----------------
```

[92]:
```
import math
import matplotlib.pyplot as plt

W=np.linspace(0.,4,100)
X=np.zeros(len(W))

for i in range(0,len(W)):
    X[i]=1-(1/math.exp(KQ0*W[i]))

plt.plot(W,X)
plt.ylabel('X')
plt.xlabel('W, kg')
```

[92]:
```
Text(0.5, 0, 'W, kg')
```



[99]:
```python
from scipy.optimize import fsolve

X=0.8
def f(W):
    return W-(math.log(1/(1-X)))/KQ0

W = fsolve(f, 0.01)
f(W)

print ('To reach', X*100, '% conversion', W, 'kg catalyst is needed.')
```

```
To reach 80.0 % conversion [3.1506601] kg catalyst is needed.
```

Q4. RTD characteristics.

RTD measurements were performed in a flow reactor with a liquid-phase reaction by a pulse tracer input. The outlet tracer concentration $(\mu mol/L)$ was measured and the equation was fit, as shown on the Figure.

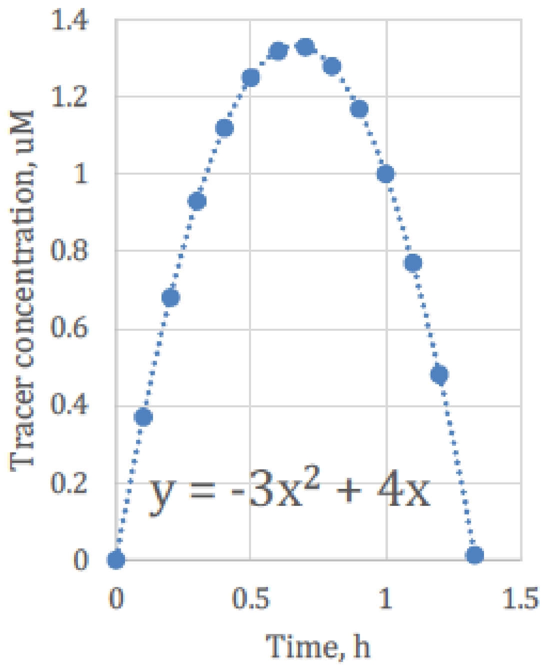
4a). Provide the algebraic equation (with all evaluated constants except for t to describe the RTD function $E(t)$.

4b). Calculate the value of cumulative distribution function $F(t)$ at $1h$. What fraction of the material will leave the reactor after $1hr$?

4c). Calculate mean residence time in this reactor (show the integration with intermediate steps; only numerical answer is not sufficient).

4d). Calculate variance of the RTD function.

4e). Assume if $50mol$ of the tracer was injected as a pulse input, and the liquid flow rate was constant at $20L/h$. Using the provided Figure, calculate if all the tracer had left by $1.5h$. Was it a wise decision to stop measurements at $1.5h$?

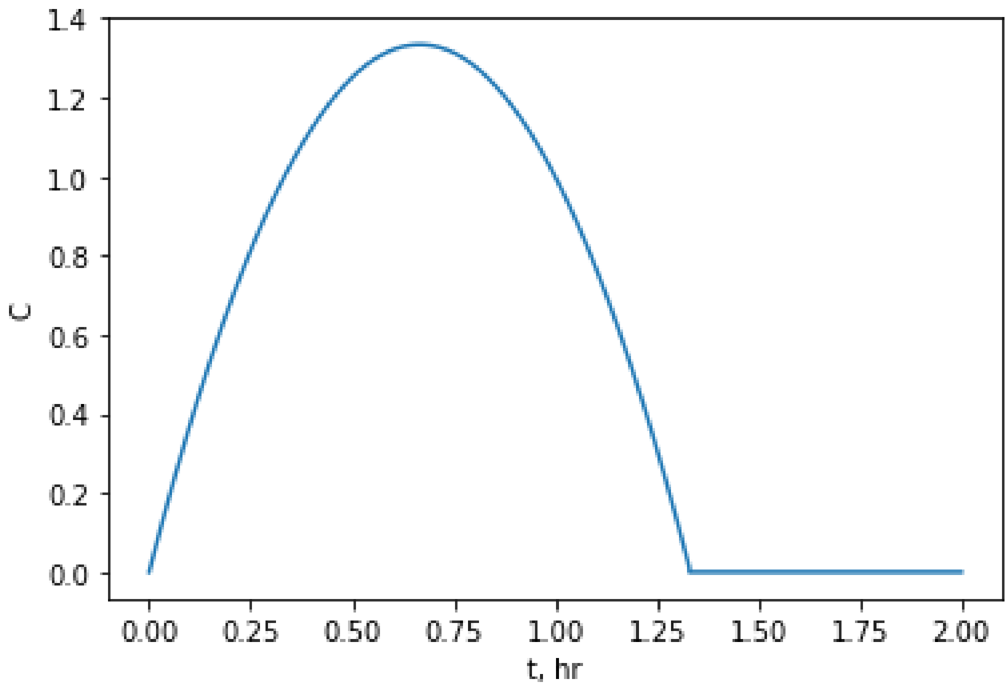


PFR.png

Answer 4a).
$c(t) = -3t^2 + 4t \quad \text{at} \quad t =< 1.33h$
$c(t) = 0 \quad\quad\quad \text{at} \quad t > 1.33h$
$\int_0^\infty c(t)dt = -3\int_0^{1.33} t^2 dt + 4\int_0^{1.33} dt = -\frac{3}{3}1.33^3 + \frac{4}{2}1.33^2 = 1.185\ (\mu M.h)$

[100]:
```
import numpy as np
import scipy.integrate as integrate

t=np.linspace(0.,2.,10000)
C=np.zeros(len(t))

for i in range(0,len(t)):
    if 0<t[i]<=1.33:
        C[i]=-3*t[i]*t[i]+4*t[i]
    else:
        C[i]=0

plt.plot(t,C)
plt.ylabel('C')
plt.xlabel('t, hr')

I = integrate.cumtrapz(C, t, initial=0)
print ("{0:.3f}".format(I[len(I)-1]))
```

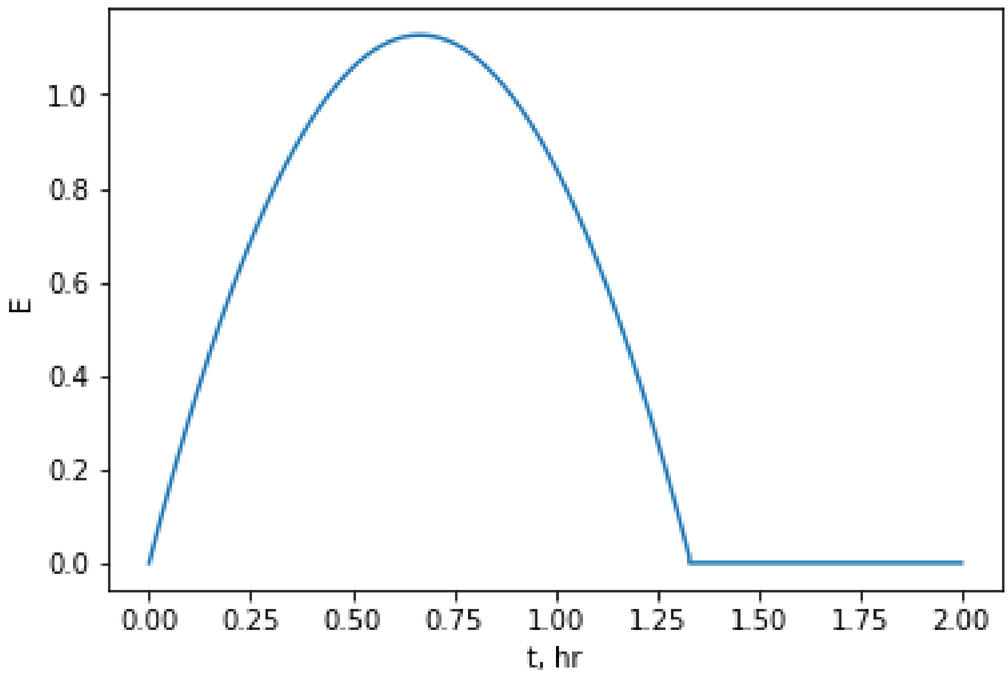
```
1.185
```



$E(t) = \frac{c(t)}{\int_0^\infty c(t)dt}$
$E(t) = -2.53t^2 + 3.376t \quad \text{at} \quad t =< 1.33h$
$E(t) = 0 \quad\quad\quad \text{at} \quad t > 1.33h$

[101]:
```
E=np.zeros(len(t))

for i in range(0,len(t)):
    if 0<t[i]<=1.33:
        E[i]=-2.53*t[i]*t[i]+3.376*t[i]
    else:
        E[i]=0
plt.plot(t,E)
plt.ylabel('E')
plt.xlabel('t, hr')
```

[101]: Text(0.5, 0, 't, hr')

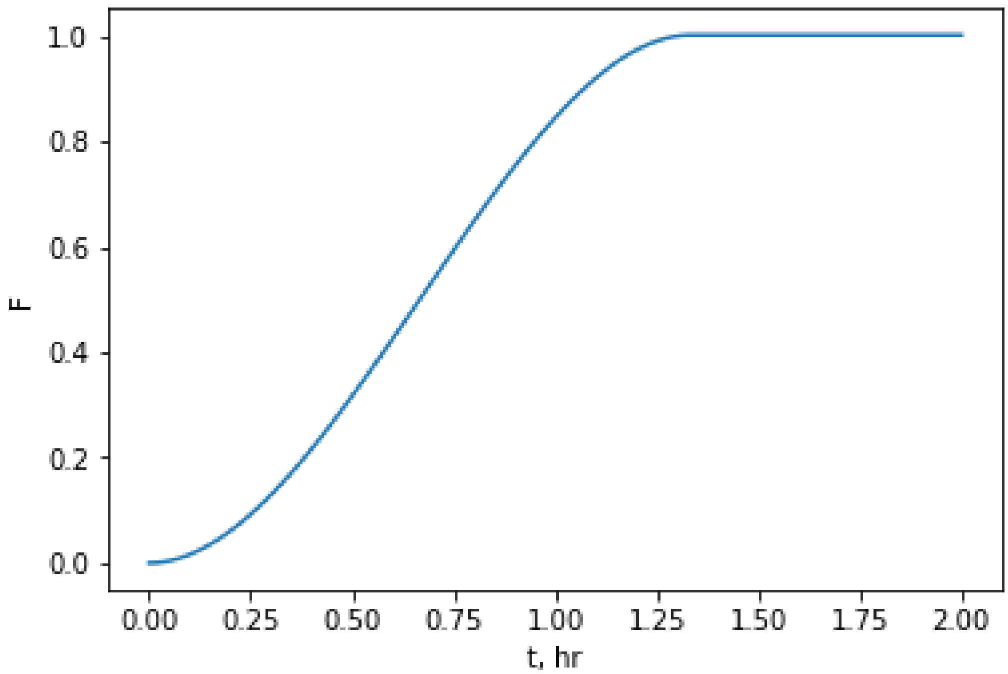


4b) $F(t) = \int_0^t E(t)dt$
at 1 hr: $F(t) = -2.53\int_0^1 t^2dt + 3.376\int_0^1 tdt = 0.845$

[106]:
```
F = integrate.cumtrapz(E, t, initial=0)

k2=0

for i in range(0,len(t)):
    if 0.99<t[i]<=1.0:
        k2=i

print ('F at t=1',"{0:.3f}".format(F[k2]))
print('Fraction leaving after 1 hr', "{0:.3f}".format(1-F[k2]))

plt.plot(t,F)
plt.ylabel('F')
plt.xlabel('t, hr')
```

```
F at t=1 0.845
Fraction leaving after 1 hr 0.155
```

[106]:
```
Text(0.5, 0, 't, hr')
```



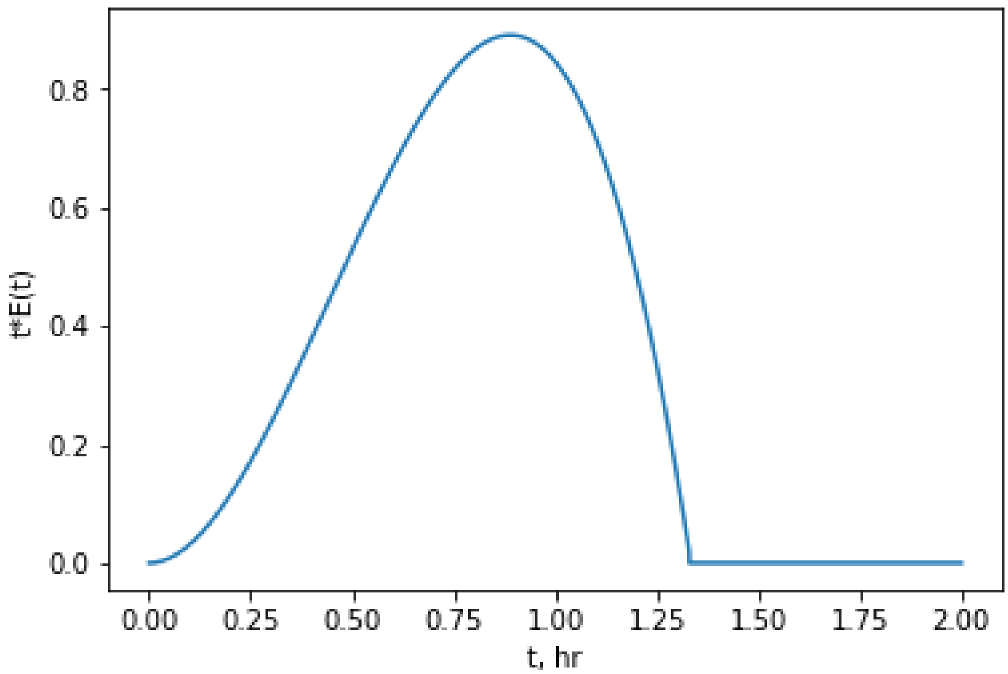
4c). Mean residence time

$$\bar{t} = \int_0^\infty tE(t)dt = -2.53\int_1^{1.33} t^3 dt + 3.376\int_0^{1.33} t^2 dt = 0.67hr$$

[78]:
```
tE=np.multiply(t,E)

tr = integrate.cumtrapz(tE, t, initial=0)
print ("{0:.3f}".format(tr[len(tr)-1]))

plt.plot(t,tE)
plt.ylabel('t*E(t)')
plt.xlabel('t, hr')
```

```
0.668
```

[78]:
```
Text(0.5, 0, 't, hr')
```



The inflection point of the parabola is at 0.67 hr
4d). Varience.
$\sigma^2 = \int_0^\infty t^2 E(t)dt - \bar{t}^2 = -2.53 \int_0^{1.33} t^4 dt + 3.376 \int_0^{1.33} t^3 dt - (0.67)^2$
$\sigma^2 = -\frac{2.53}{5} * (1.33)^5 + \frac{3.376}{4}(1.33)^4 - (0.67)^2 = 0.09h^2$

[80]:
```
v=np.zeros(len(t))

for i in range(0,len(t)):
    v[i]=t[i]*t[i]*E[i]



Va = integrate.trapz(v, t)

Var1=Va-(tr[len(tr)-1]*tr[len(tr)-1])
print ("{0:.3f}".format(Var1), 'min^2')
```

```
0.088 min^2
```

4e). The area under the curve represents the tracer left.
In **a)** we found it as $1.185\mu mol.h/L$.
Total amount of exited tracer $= C_{out} * Q = 1.185 * 20 = 23.7\mu mol$.
$50\mu mol$ is injected and not all tracer have left by $1.5h$.
We have to continue measurements and redo all calculations for $\bar{t}$ and σ^2 .

[ ]: