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Chemical Engineering Department

(0905422) Chemical Reaction Engineering II **In-Class Assessment # 1 (Chapter 7)**

Partner (1) Name: ____________________ **Partner (2) Name: __________________**

Identity (1) #: __________________ **Identity (2) #: __________________**

A process for the hydrodealkylation of toluene to produce benzene and methane has been developed. The hydrodealkylation occurs in the gas phase at high temperature and involves free radical. The free radical mechanism is believed to proceed by the sequence

Initiation: $H_2 \xrightarrow{k_1} 2H\bullet$

Propagation: $\begin{cases} H\bullet + C_6H_5CH_3 \xrightarrow{k_2} C_6H_5\bullet + CH_4 \\ C_6H_5\bullet + H_2 \xrightarrow{k_3} H\bullet + C_6H_6 \end{cases}$

Termination: $2H\bullet \xrightarrow{k_4} H_2$

The specific reaction rates k_1 and k_4 are defined w.r.t. H_2.

Derive the reaction rate law for the rate of formation of benzene based on this mechanism.

Hint: the reaction is 1/2 order in H_2 and 1st order in toluene.

(0905422) Chemical Reaction Engineering II **In-Class Assessment # 2 (Chapter 7)**

Partner (1) Name: ____________________ **Partner (2) Name: ____________________**

Identity (1) #: __________________ **Identity (2) #: __________________**

P7-6 Ozone is a reactive gas that has been associated with respiratory illness and decreased lung function. The following reactions are involved in ozone formation

$$NO_2 + h\nu \xrightarrow{k_1} NO + O$$
$$O_2 + O + M \xrightarrow{k_2} O_3 + M$$
$$O_3 + NO \xrightarrow{k_3} NO_2 + O_2$$

NO_2 is primarily generated by combustion in the automobile engine.

(a) Show that the steady-state concentration of ozone is directly proportional to NO_2 and inversely proportional to NO.

(b) In the absence of NO and NO_2, the rate law for ozone decomposition is

$$-r_{O_2} = \frac{k[O_3]^2[M]}{[O_2][M] + k'[O_3]}$$

Suggest a mechanism.

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(0905422) Chemical Reaction Engineering II	**In-Class Assessment # 7-3**
Partner (1) Name: ______________________	**Partner (2) Name:** ______________________
Partner (1) ID No.: ______________________	**Partner (2) ID No.:** ______________________

P7-11

Beef catalase has been used to accelerate the decomposition of hydrogen peroxide to yield water and oxygen. The concentration of hydrogen peroxide **is given as a function of time for a reaction mixture with a pH of 6.76 maintained at 30°C.**

t (min)	**0**	**10**	**20**	**50**	**100**
$C_{H_2O_2}$**(mol/L)**	**0.02**	**0.01775**	**0.0158**	**0.0106**	**0.005**

(a) **Determine the Michaelis-Menten parameters** V_{max} **and** K_M**.**

(b) **If the total enzyme concentration is tripled, what will** the **substrate concentration be after 20 minutes?**

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(0905422) Chemical Reaction Engineering II — **In-Class Assessment # 7-4**

Partner (1) Name: ______________________ **Partner (2) Name:** ______________________

Partner (1) ID No.: ______________________ **Partner (2) ID No.:** ______________________

For the given set of data:

(a) **Determine the Michaelis-Menten parameters V_{max} and K_M for the enzyme.**

(b) **Determine the type of inhibition, and calculate K_I.**

[S] μ M	V (no I)	V (with I)
10	4.63 nmol/min	2.70
15	5.88	3.46
20	6.94	4.74
25	9.26	6.06
30	10.78	6.49
40	12.14	8.06
50	14.93	9.71

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(0905422) Chemical Reaction Engineering II **In-Class Assessment # 10-1**

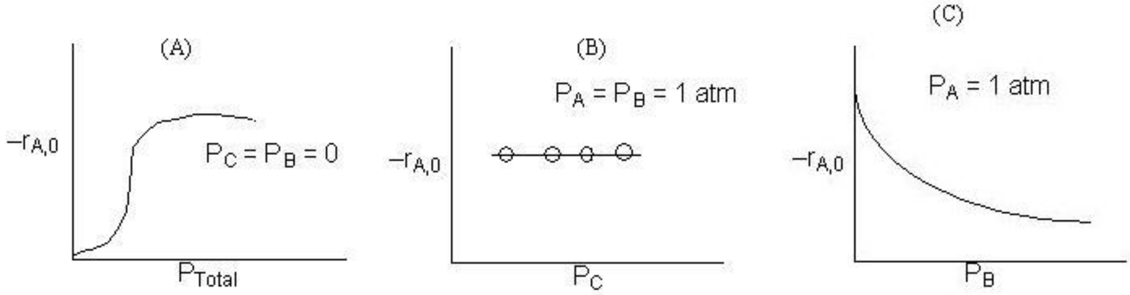
Partner (1) Name: ________________________ **Partner (2) Name:** ________________________

Partner (1) ID # ___________________________ **Partner (2) ID #** ___________________________

For the reaction:

$$A \rightleftarrows B + C$$

The initial rate of reaction is shown below



Question 1

1. The reaction is irreversible.
2. Species B is on the surface.
3. Species C is on the surface.

Choose the true one of the following:

A. 1 and 2 are true.
B. 1 and 2 are false.
C. 1 and 3 are false.
D. 2 and 3 are false.
E. 2 and 3 are true.

Question 2:
The rate law is

(A)
$$-r_A = \frac{kP_A}{1 + K_AP_A + K_BP_B}$$

(B)
$$-r_A = \frac{kP_A^2}{(1 + K_AP_A + K_CP_C)^2}$$

(C)
$$-r_A = \frac{kP_A^2}{(1 + K_AP_A + K_BP_B)^2}$$

(D)
$$-r_A = \frac{kP_A}{1 + K_AP_A + K_CP_C}$$

Question 3: Which mechanism is consistent with the rate law?

(A)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S \rightleftarrows B \bullet S + C$$

$$B \bullet S \rightleftarrows B + S$$

(B)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S \longrightarrow B + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

(C)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S + A(g) \longrightarrow B + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

(D)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S + A \bullet S \longrightarrow B + S + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

(E)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S + A \bullet S \longrightarrow B \bullet S + C + S$$

$$B \bullet S \rightleftarrows B + S$$

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(0905422) Chemical Reaction Engineering II **In-Class Assessment # 2 (Chapter 10)**

Partner (1) Name: ______________________ **Partner (2) Name: ____________________**

Partner (1) ID #: ____________________ **Partner (2) ID #: ____________________**

P10-11 Cyclohexanol was passed over a catalyst to form water and cyclohexene:

Cyclohexanol → Water + Cyclohexene

The following data were obtained.

Run	*Reaction Rate* (mol/dm^3·s) × 10^5	*Partial Pressure of Cyclohexanol*	*Partial Pressure of Cyclohexene*	*Partial Pressure of Steam (H_2O)*
1	3.3	1	1	1
2	1.05	5	1	1
3	0.565	10	1	1
4	1.826	2	5	1
5	1.49	2	10	1
6	1.36	3	0	5
7	1.08	3	0	10
8	0.862	1	10	10
9	0	0	5	8
10	1.37	3	3	3

It is suspected that the reaction may involve a dual-site mechanism, but it is not known for certain. It is believed that the adsorption equilibrium constant for cyclohexanol is around 1 and is roughly one or two orders of magnitude greater than the adsorption equilibrium constants for the other compounds. Using these data:

(a) Suggest a rate law and mechanism consistent with the data given here.

(b) Determine the constants needed for the rate law.

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(0905422) Chemical Reaction Engineering II	**In-Class Assessment # 10-3**
Partner (1) Name: ________________________	**Partner (2) Name:** ________________________
Partner (1) ID # __________________________	**Partner (2) ID #** __________________________

For the reaction:

$$2CO + O_2 \underset{cat}{\overset{\longrightarrow}{\longleftarrow}} 2CO_2$$

The following data were obtained for the oxidation of CO over a catalyst. All rates are initial rates

$-r'_{CO}$ $(mol/dm^3 \cdot s)$	C_{CO} (mol/dm^3)	C_{O_2} (mol/dm^3)
0.02	0.01	1
0.035	0.01	3
0.049	0.01	6
0.06	0.01	9
0.196	0.1	1
0.384	0.2	1
0.902	0.5	1
1.653	1	1
4.44	5	1
5.00	10	1
4.44	20	1
2.77	50	1

The initial rate was found to be independent of CO_2.

a) Suggest a rate law consistent with the data
b) Suggest mechanisms consistent with the rate law

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(0905422) Chemical Reaction Engineering II **In-Class Assessment #10-4**

Partner (1) Name: ____________ **Partner (2) Name: ____________**

Partner (1) ID #: ____________ **Partner (2) ID #: ____________**

P10-12

A recent study of the *chemical* vapor *deposition of* silica from silane (SiH_4) is believed to proceed by the following irreversible two-step mechanism:

$$SiH_4 + S \xrightarrow{k_1} SiH_2 \cdot S + H_2 \qquad (1)$$
$$SiH_2 \cdot S \xrightarrow{k_2} Si + H_2 \qquad (2)$$

This mechanism is somewhat different in that while SiH_2 is irreversibly adsorbed, it is highly reactive. In fact, adsorbed SiH_2 reacts as fast as it is formed [i.e. $r^*_{SiH2.S}$, = 0, i.e. PSSH], so that it can be assumed to behave as an active intermediate.

Determine if this mechanism is consistent with the following data:

Deposition Rate (mm/min)	***0.25***	***0.5***	***0.75***	***0.80***
Silane Pressure (mtorr)	**5**	**15**	**40**	**60**

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(0905422) Chemical Reaction Engineering II	**In-Class Assessment #10-5**
Partner (1) Name: ________________	**Partner (2) Name:** ________________
Partner (1) ID #: ________________	**Partner (2) ID #:** ________________

P10-13

Vanadium oxides are of interest for various sensor applications, owing to the sharp metal–insulator transitions they undergo as a function of temperature, pressure, or stress. Vanadium triisopropoxide (VTIPO) was used to grow vanadium oxide films by *chemical vapor deposition* [*J. Electrochem. Soc.*, *136*, 897 (1989)]. The deposition rate as a function of VTIPO pressure for two different temperatures follows:

$T = 120°C$:

Growth Rate (μm/h)	0.004	0.015	0.025	0.04	0.068	0.08	0.095	0.1
VTIPO Pressure (torr)	0.1	0.2	0.3	0.5	0.8	1.0	1.5	2.0

$T = 200°C$:

Growth Rate (μm/h)	0.028	0.45	1.8	2.8	7.2
VTIPO Pressure (torr)	0.05	0.2	0.4	0.5	0.8

In light of the material presented in this chapter, analyze the data and describe your results. Specify where additional data should be taken.

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(0905422) Chemical Reaction Engineering II | **In-Class Assessment # 13-2**

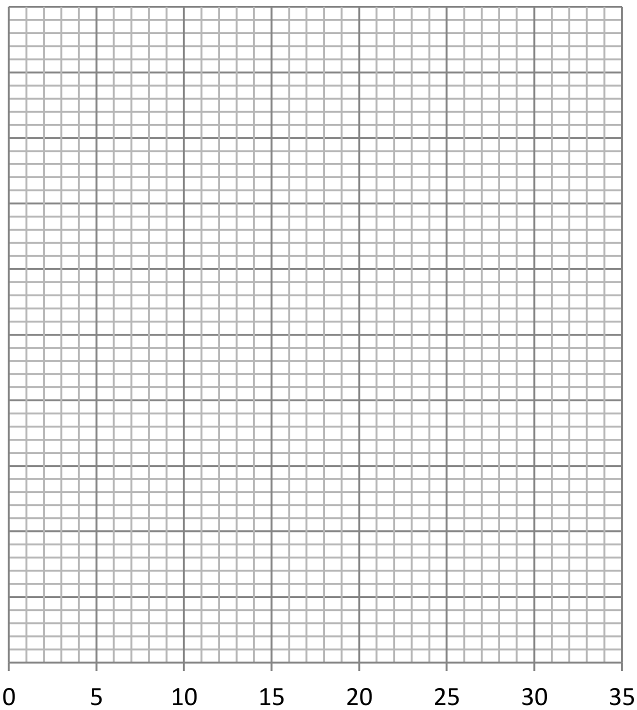
Partner (1) Name: ____________________ **Partner (2) Name: ____________________**

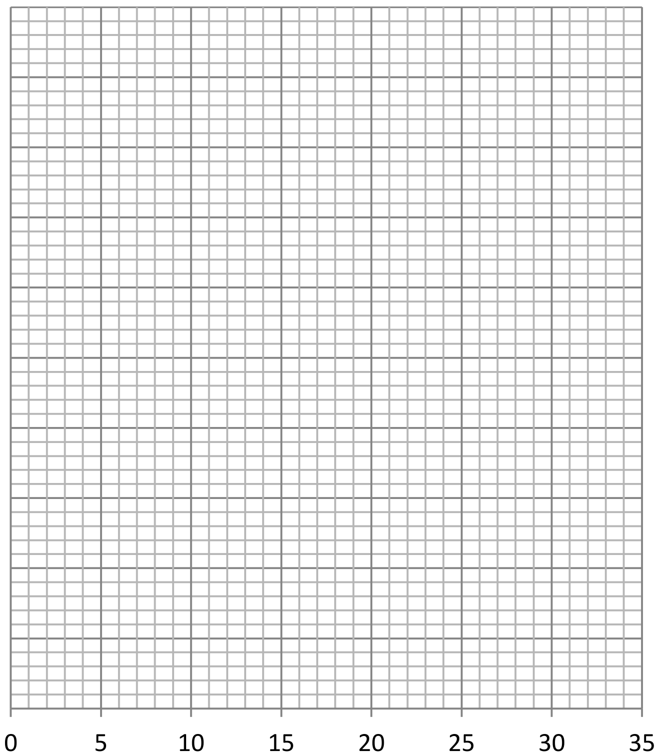
Partner (1) ID #: ____________________ **Partner (2) ID #: ____________________**

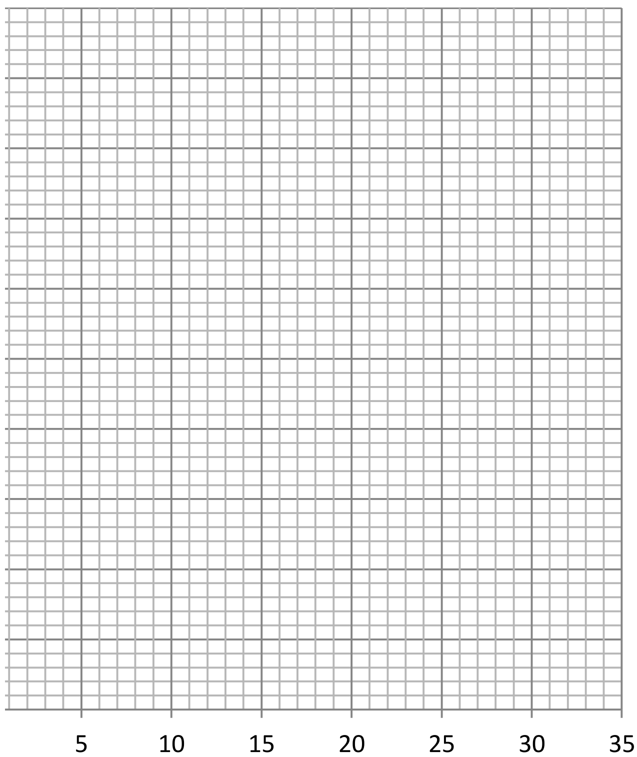
The following data were obtained from a tracer test to a reactor.

t(s)	0	5	10	15	20	25	30	35
C_t (mg/dm^3)	0	0	0	5	10	5	0	0

1) Plot $C_t(t)$.
2) Find $E(t)$.
3) Find the fraction of material that spends between 15 and 20 seconds in the reactor.
4) Find F(t) and, the fraction of material that spends 25 seconds or less in the reactor.
5) Evaluate mean residence time.
6) Evaluate the variance.







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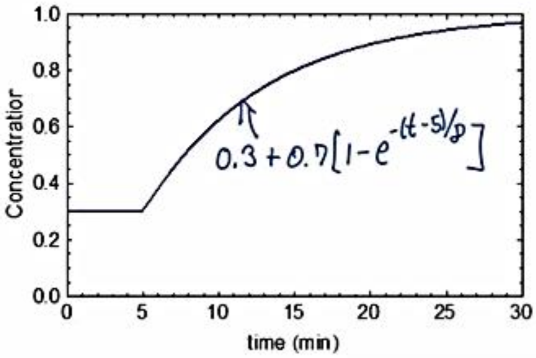
(0905422) Chemical Reaction Engineering II	**In-Class Assessment # 13-3**
Partner (1) Name: ________________________	**Partner (2) Name:** ________________________
Partner (1) ID No.: ________________________	**Partner (2) ID No.:** ________________________

Model non-ideal CSTR

A non-ideal, continuous stirred tank reactor (CSTR) has the normalized response to a step function input of a tracer shown in the figure. The step input starts at t = 0.



a) Develop a 3-parameter model of this non-ideal reactor. The model can consist of ideal reactors, recycle, bypass, and hold-up,

b) Determine the values of the parameters for the model. The total reactor volume is 1.5 L and the inlet volumetric feedrate is O. 10 L/min.

c) Sketch the exit age distribution for the non-ideal reactor.

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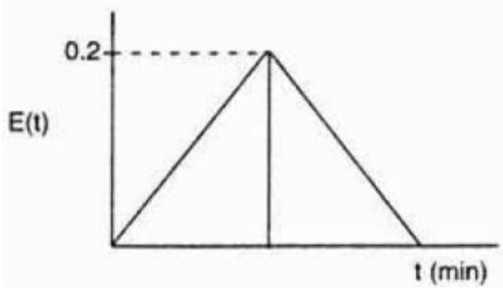
(0905422) Chemical Reaction Engineering II	**In-Class Assessment # 13-4**
Name: ________________________	**Partner Name: ________________________**
ID # ______________________	**Partner ID # ______________________**

P13-6
The following E(t) curve was obtained from a tracer test on a tubular reactor in which dispersion is believed to occur.

A second-order reaction
$A \xrightarrow{k} B$ with $kC_{A0} = 0.2 \text{ min}^{-1}$
is to be carried out in this reactor. There is no dispersion occurring either upstream or downstream of the reactor, but there is dispersion inside the reactor.



(a) What is the mean residence lime t_m?
(b) What is the variance σ^2?
(c) What conversions do you expect from an ideal PFR and an ideal CSTR in a real reactor t_m?
(d) What is the conversion predicted by
  1) the segregation model?
  2) the maximum mixedness model**?**

The CSTR

- Concentration $C(t) = C_0 e^{-t/\tau}$
- RTD Function $E(t) = \frac{e^{-t/\tau}}{\tau}$
- Cumulative Function $F(t) = 1 - e^{-t/\tau}$
- Space Time $\tau = \frac{V}{v_0}$

a. Perfect Operation (P)

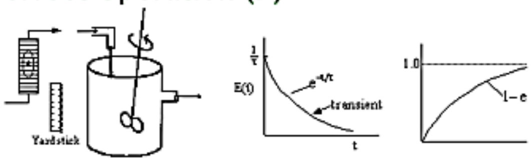


Figure 13-11 Perfect operation of a CSTR.

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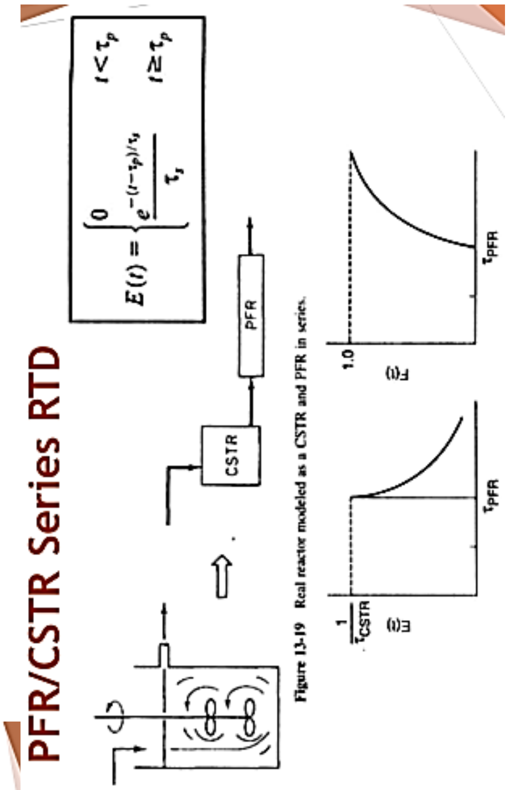

b. Bypassing (BP)

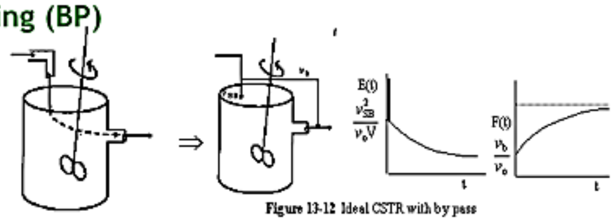

Figure 13-12 Ideal CSTR with by pass

- A volumetric flow rate, v_b, bypasses the reactor while a volumetric flow rate v_{SB} enters the system volume and ($v_0 = v_b + v_{SB}$).
- The reactor system volume V_s is the well-mixed portion of the reactor.
- $v_{SB} < v_0 \Rightarrow \tau_{SB} > \tau$ $\quad E(t) = \frac{v_b}{v_0}\delta(t-0) + \frac{v_{SB}^2}{V v_0} e^{-t/\tau_{SB}}$

c. Dead Volume (DV)

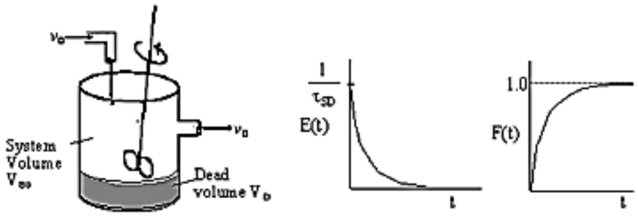

Figure 13-13 Ideal CSTR with dead volume

- The total volume, V, is the same as that for perfect operation, with $V = V_D + V_{SD}$.
- $V_{SD} < V \Rightarrow \tau_{SD} < \tau$

Summary