Name: _____ KEY _____ **gtID#** _____

ChBE 4300A – Kinetics and Reactor Design
Exam #2 – April 1st, 2014 – 2 hours – Closed Book
School of Chemical & Biomolecular Engineering
Georgia Institute of Technology
Prof. Michael A. Filler
Spring 2014

Problem #1		/30
Problem #2		/35
Problem #3		/35
Total		**/100**

I have read the Georgia Institute of Technology Academic Honor code. I understand and accept my responsibility as a member of the Georgia Tech Community to uphold the Academic Honor Code at all times.

**Signature:** _____ **Date:** _____

Remember:
- No wireless devices are permitted at any time.
- Show all of your work.
- Explain your reasoning and state all assumptions.
- Additional worksheets are available if necessary.

Useful Constants:

Avagadro's constant	L	6.022×10^{23} molecules/mol
Universal gas constant	R	1.987 cal/mol-K = 8.314 J/mol-K
Boltzmann's constant	k_B	1.381×10^{-23} J/K

Problem 1. (30 points)   **Name:** <u>KEY</u>

Consider two isothermal reactors in series, specifically a PFR followed by a CSTR, where a liquid-phase reaction is taking place:

$$A \rightarrow \text{products}$$
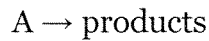
You already know that the kinetic rate expression exhibits a classic power law dependence and previous experiments gave you a value for the rate constant, k:

$$r_A = -kc_A^n$$

However, you still do not know the reaction order, n.

You colleague has run a series of experiments where the inlet concentration of A (at the PFR), C_{Ao}, was varied and the outlet concentration of A (at the CSTR), C_{A2}, was measured at steady-state. **Assuming a constant reactor space time, τ, how would you plot the data collected by your colleague in order to extract the reaction order?**

$\underline{\text{PFR}}: \quad \dfrac{dC_A}{d\tau_1} = -kC_A^n$

$\displaystyle\int_{C_{Ao}}^{C_{A1}} \dfrac{dC_A}{C_A^n} = -k \int_0^{\tau_1} d\tau$

$\dfrac{1}{1-n}\left[C_{A1}^{1-n} - C_{Ao}^{1-n} \right] = -k\tau_1$

$C_{A1}^{1-n} = C_{Ao}^{1-n} - (1-n)k\tau_1$

$C_{A1} = \left[C_{Ao}^{1-n} - (1-n)k\tau_1 \right]^{1/1-n}$

$\underline{\text{CSTR}}: \quad F_{A1} - F_{A2} + r_A V = 0$

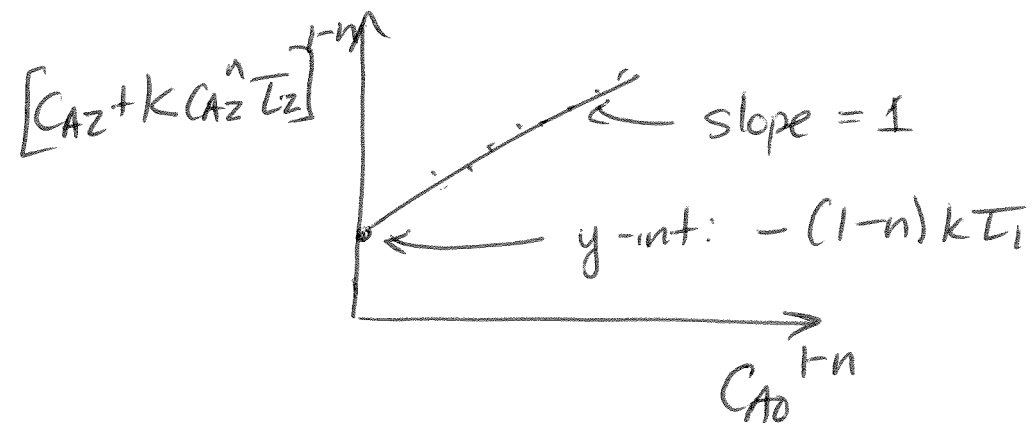$\quad\quad\quad\quad C_{A1} - C_{A2} - kC_{A2}^n \tau_2 = 0$

Substituting for C_{A1}:

$\left[C_{Ao}^{1-n} - (1-n)k\tau_1 \right]^{1/1-n} = C_{A2} + kC_{A2}^n \tau_2$

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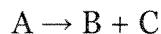$$\underbrace{C_{A0}^{1-n}}_{mx} \underbrace{-(1-n)k\bar{t}_1}_{b} = \underbrace{\left[C_{A2} + kC_{A2}^{n}\bar{t}_2\right]^{1-n}}_{y}$$

$\left[C_{A2} + kC_{A2}^{n}\bar{t}_2\right]^{1-n}$

slope $= 1$

y-int: $-(1-n)k\bar{t}_1$

C_{A0}^{1-n}

→ vary n until data yields straight line

→ extract n via y-intercept

✗✗ several variations on this general idea were accepted.

The liquid-phase reaction

$$A \to B + C$$

is being studied in an isothermal CSTR with a space time of 1 min. The reaction is first-order with respect to A and exhibits a rate constant of 1 min^{-1}. The reactor is initially operating at steady-state with a feed concentration of A equal to 1 mol/m^3. The feed concentration is suddenly changed to 2 mol/m^3, with all other parameters held constant. **Calculate the effluent composition 1 min after the change in the input composition.**

$$\frac{d(C_A V)}{dt} = C_{A0} \nu_0 - C_A \nu_0 - k C_A V$$

$$\frac{dC_A}{dt} = \underbrace{\frac{C_{A0}}{\tau}}_{\equiv a} - \underbrace{\left(\frac{1}{\tau} + k\right) C_A}_{\equiv b} = a - b C_A$$

Integrating via separation of variables:

transient $\to$

$$\int_{C_{A,ss}}^{C_{A,T}} \frac{dC_A}{a - b C_A} = \int_0^t dt$$

↑ Steady-state

$$-\frac{1}{b} \ln(a - b C_A) \Big|_{C_{A,ss}}^{C_{A,T}} = t$$

$$\ln\left(\frac{a - b C_{A,T}}{a - b C_{A,ss}}\right) = -bt$$

$$C_{A,T} = \frac{1}{b}\left[a - e^{-bt}(a - b C_{A,ss})\right]$$

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Need $C_{A,SS} = \dfrac{C_{A0,SS}}{1+k\bar{\tau}} = \dfrac{1}{2}$ ← original feed

$$a = \dfrac{C_{A0}}{\bar{\tau}} = \dfrac{2}{1} = 2 \quad \leftarrow \text{new feed}$$

$$b = \dfrac{1}{\bar{\tau}} + k = 2$$

Substituting:

$$C_{A,T} = \dfrac{1}{2}\left[2 - e^{-2}\left(2 - 2\left(\dfrac{1}{2}\right)\right)\right]$$

$$= \dfrac{1}{2}\left[2 - e^{-2}\right]$$

$$\boxed{C_{A,T} = 0.93 \ mol/m^3}$$
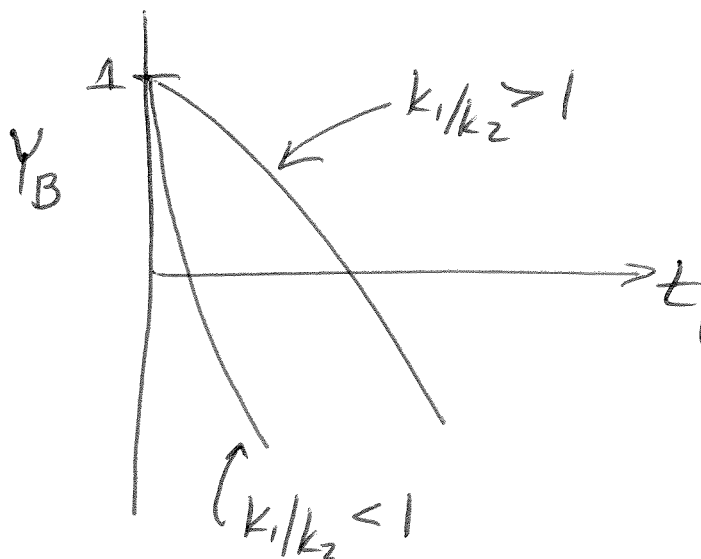
You are tasked with designing an isothermal PFR to carry out the following set of first-order series reactions at steady-state:

$$A \rightarrow B \qquad k_1$$
$$B \rightarrow C \qquad k_2$$

The feed is pure A.

(a) Qualitatively plot the instantaneous yield of B as a function of ~~time~~ space for several values of k_1/k_2. Explain the result.

① @ start, $C_B = 0$

$$Y_B \approx \frac{k_1 C_A}{k_1 C_A} = 1$$

② as time progresses $C_B \uparrow$

$$Y_B = \frac{k_1 C_A - k_2 C_B}{k_1 C_A \uparrow} < 1$$

increasing in magnitude

③ eventually

$$Y_B = \frac{k_1 C_A - k_2 C_B}{k_1 C_A} < 0$$

(after C_B passes through a maximum)

(b) What reactor space time, τ, maximizes the concentration of species B. Your answer should only be a function of k_1 and k_2.

$$\frac{dC_A}{d\tau} = -k_1 C_A \implies C_A = C_{A0} e^{-k_1 \tau}$$

$$\frac{dC_B}{d\tau} = k_1 C_A - k_2 C_B$$

$$\frac{dC_B}{d\tau} + k_2 C_B = k_1 C_{A0} e^{-k_1 \tau}$$

use an integrating factor to solve $y' + p(t)y = f(t)$

$$I = e^{\int k_2 d\tau} = e^{k_2 \tau}$$

$$C_B = e^{-k_2 \tau} \left[\int e^{k_2 \tau'} e^{-k_1 \tau'} k_1 C_{A0} d\tau' + C \right]$$

integrating yields

$$C_B = e^{-k_2 \tau} \left\{ \frac{k_1 C_{A0}}{k_2 - k_1} e^{(k_2 - k_1)\tau} + C \right\}$$

apply I.C. $C_B = 0$ @ $\tau = 0 \implies C = -\frac{k_1 C_{A0}}{k_2 - k_1}$

$$C_B = \frac{k_1 C_{A0}}{k_2 - k_1} \left(e^{-k_1 \tau} - e^{-k_2 \tau} \right)$$

(c) For $k_1/k_2 \gg 1$, do you expect the <u>maximum concentration of B</u> for a <u>CSTR</u> with the same set of reactions and inlet conditions to change? If so, would it increase or decrease? How about for $k_1/k_2 \ll 1$? Explain your reasoning.

For $k_1/k_2 \gg 1$, <u>no difference</u> in $c_{B,max}$ since second reaction is so slow

(i.e. easy to "stop" on B)

For $k_1/k_2 \ll 1$, <u>no difference</u> in $c_{B,max}$ since second reaction is so fast

(i.e. no reactor is able to effectively "stop" on B)

(b) continued

$$\frac{dc_B}{d\tau} = 0 \quad \text{gives optimum } \tau \text{ (and } c_B)$$

$$0 = \frac{c_{A0}k_1}{k_2 - k_1}\left(-k_1 e^{-k_1\tau} + k_2 e^{-k_2\tau}\right)$$

$$k_1 e^{-k_1\tau} = k_2 e^{-k_2\tau}$$

$$k_1/k_2 = e^{(k_1 - k_2)\tau}$$

$$\boxed{\tau_{s,opt} = \frac{\ln k_1/k_2}{k_1 - k_2}}$$

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