Exam 2
Chemical Reaction Engineering
20 April 2000
Closed Book and Notes

(40 pts) 1). You have been asked by your boss to design a reactor for a liquid phase cracking reaction. Your boss believes that this reaction can be conducted in one of the CSTR's that is currently not being used at the refinery. You have available three CSTR's which are summarized in the table below:

CSTR	Volume (m^3)	Heat Transfer Area (m^2)
1	6.28	17.3
2	6.28	12.6
3	17.67	15.5

a) Which reactor would you recommend using for the cracking process?
b) Determine the conversion of A for your recommended reactor using the graphical method. Note the conversion from the mole balance for each reactor has been plotted on the graph on the next page. Note that reactors 1 and 2 give identical conversions.

$\mathrm{A} \rightarrow \mathrm{B} + \mathrm{C}$ Elementary Reaction

$F_{A0} = 4000 \text{ mol/hr}$

$F_{B0} = F_{C0} = 0$

$Q_0 = 20.94 \text{ m}^3\text{/hr}$

$T_0 = 450 \text{ K}$ (Feed Temperature)

$\Delta H^{\circ}_{rxn}\Big|_{T_R=298K} = 80{,}000 \text{ J/(mol A)}$

$C_{pA} = 245.4 \text{ J/(mol K)}$

$C_{pB} = 120 \text{ J/(mol K)}$

$C_{pC} = 125.4 \text{ J/(mol K)}$

Reaction Rate Parameters:

$k = 6.899 \times 10^{-8} \text{ hr}^{-1}$ at 298 K

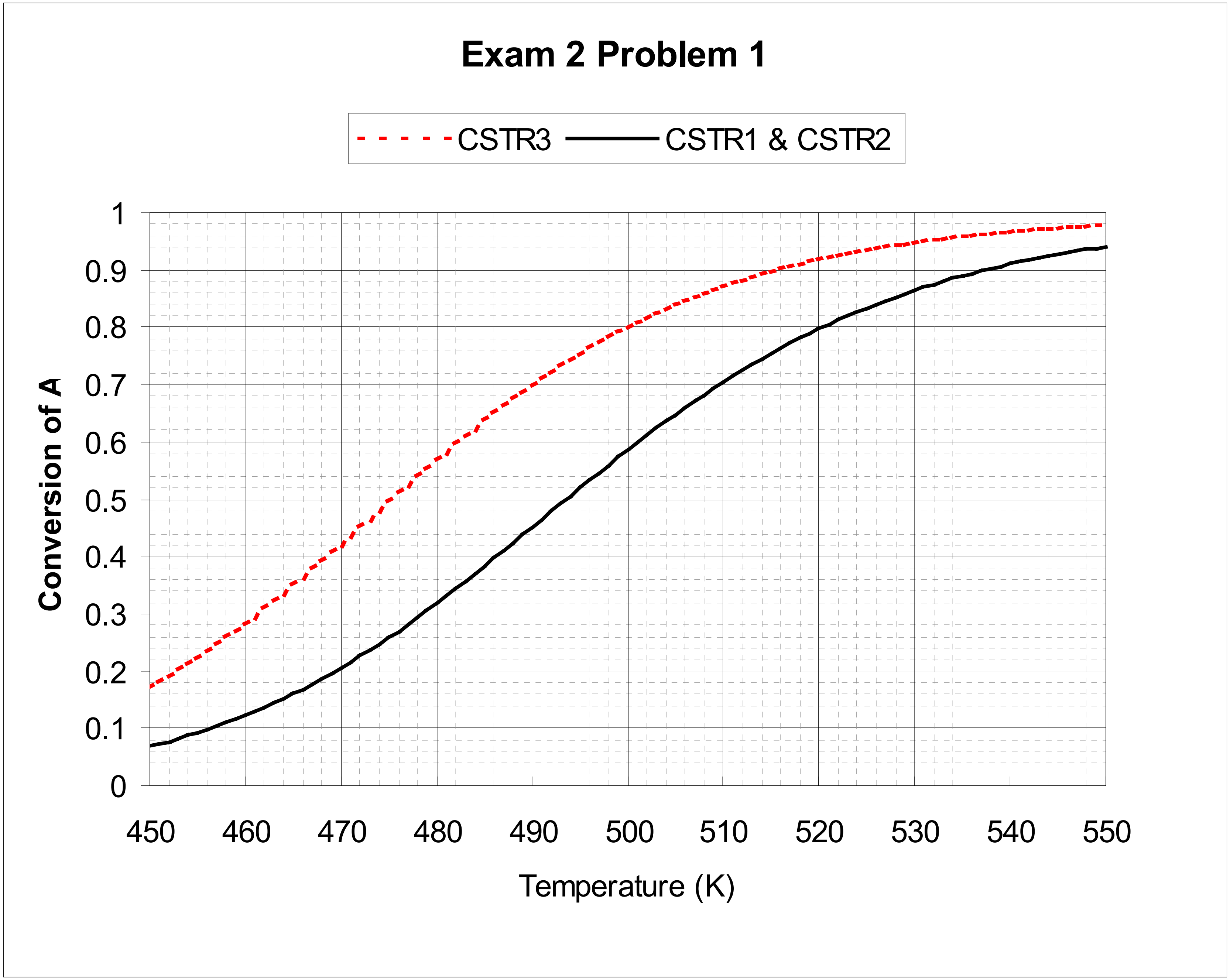
$E_a = 110{,}626 \text{ J/mol}$ (Activation Energy)

$R = 8.314 \text{ J/(mol K)}$

Heat Transfer Terms

$U = 80{,}000 \text{ J/(hr m}^2\text{ K)}$

$T_a = 700 \text{ K}$


Exam 2 Problem 1
CSTR3
CSTR1 & CSTR2
Conversion of A
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
450
460
470
480
490
500
510
520
530
540
550
Temperature (K)

(50) Problem 1. Exam A

$A \rightarrow B + C$ liquid phase

X_{MB} given

$0 = F_{A_0} - F_A + r_A V$

$0 = F_{A_0} X_A + r_A V$

E.B. $0 = 0 + \dot{Q} - \sum F_{i0} C_{p_i} (T - T_0) + \Delta H_{rxn} (-F_{A_0} X_A)$

$\dot{Q} = UA(T_a - T)$

$\Delta H_{rxn}|_T = \Delta H_{rxn}|_{T_R} + \Delta C_p (T - T_R)$

$\Delta C_p = C_{p_B} + C_{p_C} - C_{p_A}$

$= 120 + 125.4 - 245.4 = 0$

$$\frac{-\dot{Q}}{4000 \frac{mol}{hr}} + \sum \left(4000 \frac{mol}{hr}\right)\left(245.4 \frac{J}{mol\,K}\right)(T - T_0) = \left(-80{,}000 \frac{J}{mol}\right) 4000 \frac{mol}{hr} X$$

$$-\frac{\left(80{,}000 \frac{J}{hr\,m^2 K}\right)(A)(700K - T)}{4000\ mol/hr} + 245.4(T - T_0) = -80{,}000 \frac{J}{mol\,A} X$$

CSTR 1 $-(20)(17.3) \frac{J}{K\,mol} (700K - T) + 245.4(T - T_0) = -80000 X \frac{J}{mol}$

$T \left[(+20)(17.3) \frac{J}{K\,mol} + 245.4 \frac{J}{mol\,K}\right] / -80{,}000\ J/mol$

$\left[-(20)(17.3)(700) \frac{J}{mol} - 245.4(450K)\right] / (-80{,}000) = X$

$T(+0.00739\ 1/K) + 4.41 = X$

at $T = 540$ $X = 0.416$

$T = 450$

SS soln $X = 0.664$ $T = 506K$

Exam A

RSTR 2

$T(-0.00622) + 3.585 = X$

T	X
490	0.54
530	0.29

SS soln $X = 0.511$ $T = 494$

CSTR 3

$T(-0.00644) + 4.093 = X$

T	X
530	0.413

SS Soln $X = 0.694$ $T = 490K$

CSTR 3 $(A = 15.5 m^2)$ is the best with the highest conversion at $X = 0.695$ $T = 490K$

<u>for exam A</u> 16.5 min

Exam B:

CSTR 1 $X = 0.664$ $T = 506$ <u>Highest X</u>

CSTR 1	$A = 17.3 m^2$	Same as A	$X = 0.664$	$T = 506 K$
CSTR 2	$A = 12.6 m^2$	Same as A	$X = 0.511$	$T = 494K$
CSTR 3	$A = 13.9 m^2$		$X = 0.638$	$T = 485$

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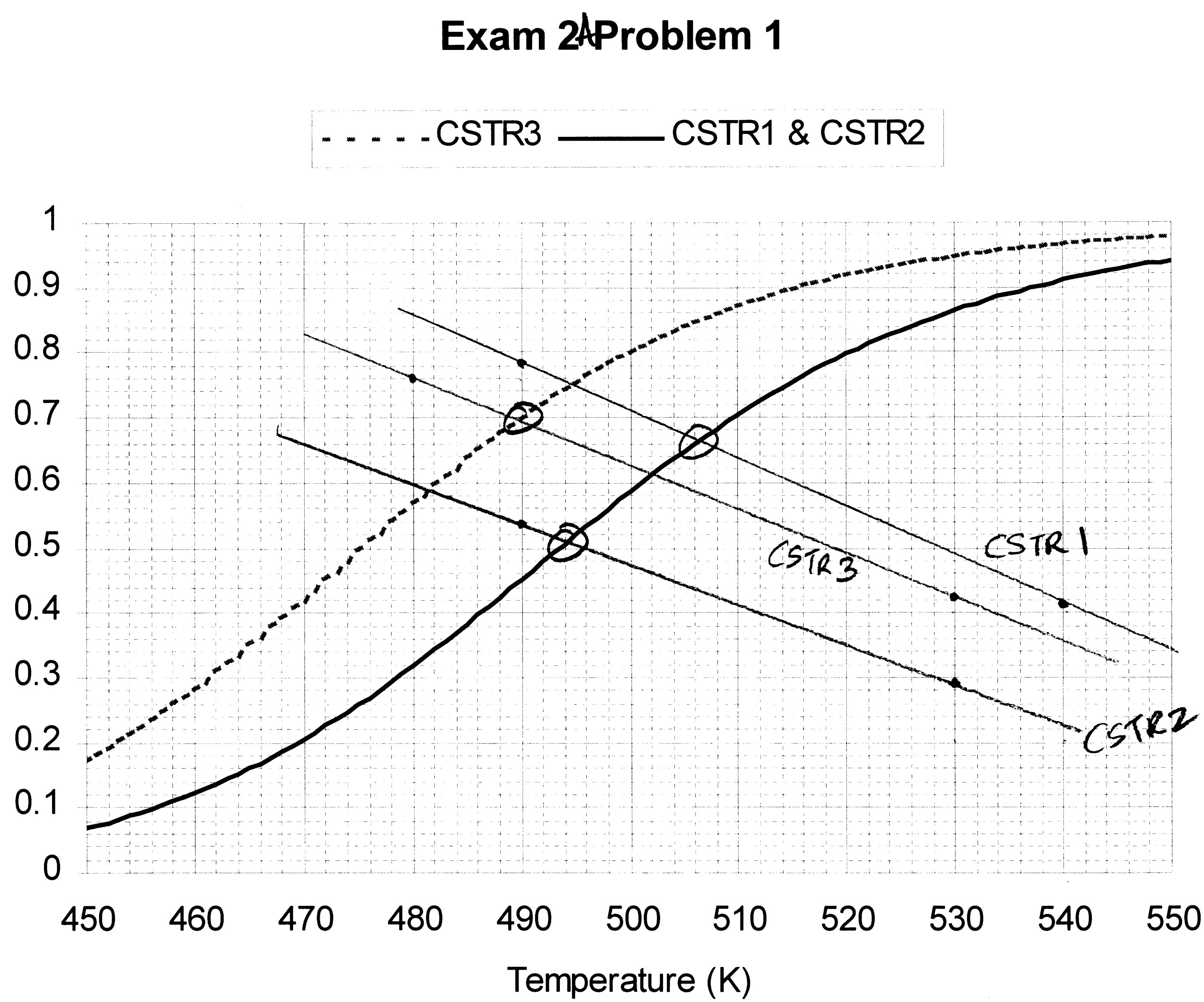

Exam 2A Problem 1
CSTR3
CSTR1 & CSTR2
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
450
460
470
480
490
500
510
520
530
540
550
Temperature (K)
CSTR 1
CSTR 3
CSTR2

Not required:

Mole Balance

$$0 = F_{A0} - F_A + r_A V$$

$$0 = F_{A0} - F_A + (-kC_A)V$$

liquid phase $\varphi = \varphi_0$ $\quad F_A = C_A \varphi$

$$0 = C_{A0}\varphi_0 - C_A\varphi - kC_A V$$

$$x_A \equiv \frac{F_{A0} - F_A}{F_{A0}} = \frac{C_{A0}\varphi_0 - C_A\varphi}{C_{A0}\varphi_0} \underset{\substack{\text{for liquid phase} \\ \varphi_0 = \varphi}}{=} \frac{C_{A0} - C_A}{C_{A0}}$$

$$\therefore \quad C_A = C_{A0}(1 - x)$$

$$0 = C_{A0}\varphi_0 - C_{A0}\varphi_0(1-x) - kC_{A0}(1-x)V$$

$$0 = \varphi_0 - \varphi_0(1-x) - k(1-x)V$$

$$\varphi_0 = \varphi_0(1-x) + k(1-x)V = (1-x)\left[\varphi_0 + kV\right]$$

$$1 - x = \frac{\varphi_0}{\varphi_0 + kV}$$

$$x = 1 - \frac{\varphi_0}{\varphi_0 + kV} = \frac{\varphi_0 + kV - \varphi_0}{\varphi_0 + kV} = \frac{kV}{\varphi_0 + kV}$$

$$x = \frac{1}{\varphi_0/kV + 1} = \frac{1}{1/\tau k + 1} \text{ or } \frac{\tau k}{1 + \tau k}$$

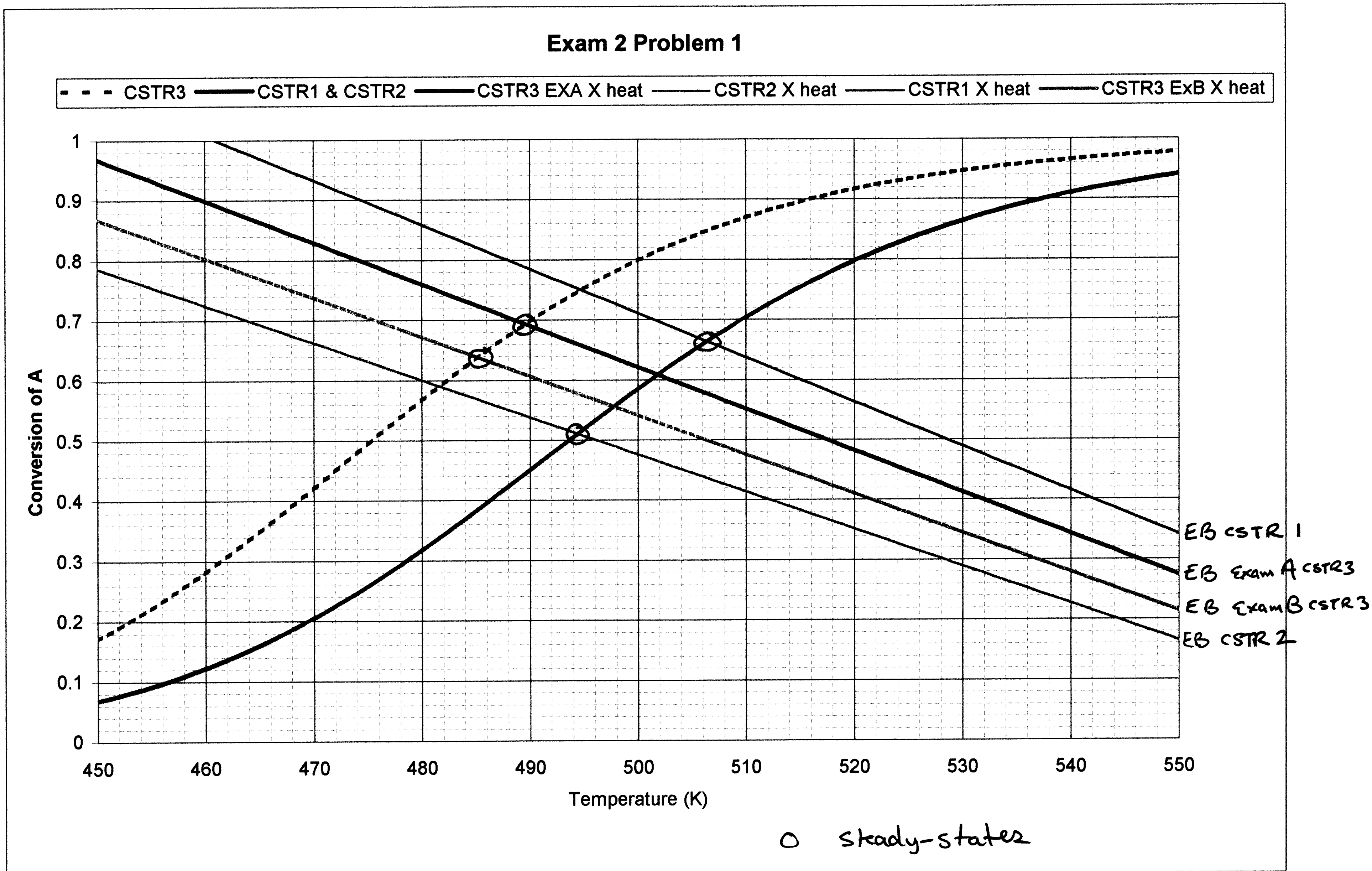
with $\tau = \frac{V}{\varphi_0}$

if plugging in $r_A V$ into E.B. $\quad r_A V = -kC_A V = -kC_{A0}V(1-x)$

Not Required

finding A $\quad k = A\exp(-E/RT)$

$$\frac{(6.899 \times 10^{-8}\,hr^{-1})}{\exp\left(-\frac{110{,}626}{8.314\,\frac{J}{mol\,K}}\frac{1}{298K}\right)} = A = 1.7 \times 10^{12}\,hr^{-1}$$



Exam A x = CSTR 3

Exam B x = CSTR 1