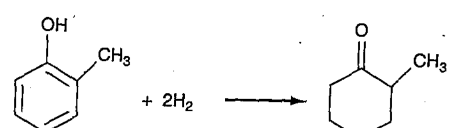
rently 14.1% conversion is realized. The entering pressure is 20 atm and the pressure at the exit of the reactor is 9.0 atmospheres. It is believed that this reaction is internal diffusion limited. We know from Chapter 12 of Elements of CRE (e.g. P4-23$_C$ or Eqn. 12-35, page 751) that for internal diffusion limitations the rate of reaction varies inversely with the catalyst particle size. Consequently one of the engineers suggests that the catalyst be ground up into a smaller size. She also notes the smallest size to which the catalyst may be ground is 0.01 cm. and that there are 3 other pipe sizes available into which the catalyst could be packed. These non-corrosive heat-resistant pipes, which can be cut to any length, are 2 cm, 3 cm, and 6 cm in diameter.

(a) Calculate the maximum value of the pressure drop parameter, α, that you can have and still maintain an exit pressure of 1 atm. (*Ans.*: $\alpha = 9.975 \times 10^{-4}$ kg.)
(b) What conversion could be achieved in a CSTR with the same catalyst weight and no ΔP? (*Ans.*: $X = 0.18$.)
(c) Should you change the catalyst size and pipe diameter in which 1000 kg of the catalyst is packed while maintaining the catalyst weight?
(d) Next consider how α would change if you changed both pipe size and particle size. Can you change pipe size and particle size at the same time such that α remains constant at the value calculated in part (c)?
(e) For the conditions of part (a) [i.e., maintain α constant at the value in part (a)], pick a pipe size and calculate a new particle size. (*Ans.*: $D_P = 0.044$ cm.)
(f) Calculate a new specific reaction rate ratio assuming (i.e., recall the effectiveness factor from Chapter 12) that

$$k \sim \frac{1}{D_P} \quad \text{then} \quad k_2 = k_1 \left(\frac{D_{P1}}{D_{P2}}\right)$$

(g) Using the new values of k and α, calculate the conversion for a PBR for the new particle size for an exit pressure of 1 atm. (*Ans.*: $X = 0.78$.)

P4-22$_B$ Alkylated cyclohexanols are important intermediates in the fragrance and perfume industry [*Ind. Eng. Chem. Res.*, *28*, 693 (1989)]. Recent work has focused on gas-phase catalyzed hydrogenation of *o*-cresol to 2-methylcyclohexanone, which is then hydrogenated to 2-methylcyclohexanol. In this problem we focus on only the first step in the reaction (Figure P4-22). The reaction on a nickel–silica catalyst was found to be zero-order in o-cresol and first-order in hydrogen with a specific reaction rate at 170°C of 1.74 mol of *o*-cresol/(kg cat · min · atm). The reaction mixture enters the packed-bed reactor at a total pressure of 5 atm. The molar feed consists of 67% H_2 and 33% *o*-cresol at a total molar rate of 40 mol/min.



No ΔP
r_A W
C_i W
with ΔP
explore

(a) [redacted] plot the rate of reaction of *o*-cresol and the concentrations of each species as a function of catalyst weight. What is the ratio of catalyst weight needed to achieve the last 5% conversion to the weight necessary to achieve the first 5% conversion (0 to 5%) in the plug-flow reactor?
(b) Accounting for the pressure drop in the packed bed using a value of $\alpha = 0.34$ kg^{-1}, redo part (a) along with a plot of pressure versus catalyst weight.
(c) Another engineer suggests that instead of changing catalyst size it would be better to pack the catalyst in a shorter reactor with twice the pipe diameter. If all other conditions remain the same, is this suggestion better?

P4-23$_C$ The elementary gas-phase reaction

$$A + B \longrightarrow C + D$$

is carried out in a packed-bed reactor. Currently, catalyst particles 1 mm in diameter are packed into 4-in. schedule 40 pipe ($A_C = 0.82126$ dm^2). The value of β_0 in the pressure drop equation is 0.001 atm/dm. A stoichiometric mixture of A and B enters the reactor at a total molar flowrate of 10 gmol/min, a temperature of 590 K, and a pressure of 20 atm. Flow is turbulent throughout the bed. Currently, only 12% conversion is achieved with 100 kg of catalyst.

It is suggested that conversion could be increased by changing the catalyst particle diameter. Use the data below to correlate the specific reaction rate as a function of particle diameter. Then use this correlation to determine the catalyst size that gives the highest conversion. As you will see in Chapter 12, k' for first-order reaction is expected to vary according to the following relationship

$$k' = \eta k = \frac{3}{\Phi^2}(\Phi \coth \Phi - 1)\, k \qquad \text{(P4-23.1)}$$

where Φ varies directly with particle diameter, $\Phi = cd_p$. Although the reaction is not first-order, one notes from Figure 12-5 the functionality for a second-order reaction is similar to Equation (P4-23.1). (*Ans.*: $c = 75$)
(a) Make a plot of conversion as a function of catalyst size.
(b) Discuss how your answer would change if you had used the effectiveness factor for a second-order reaction rather than a first-order reaction.
(c) Discuss what you learned from this problem and what you believe to be the point of the problem.

Additional information:
Void fraction = 0.35 Bulk catalyst density = 2.35 kg/dm^3

Catalyst Diameter, d_p (mm)	2	1	0.4	0.1	0.02	0.002
k' (dm^6/mol · min · kg cat)	0.06	0.12	0.30	1.2	2.64	3.00

[*Hint*: You could use Equation (P4.23-1), which would include d_P and an unknown proportionality constant which you could evaluate from the data. For very small values of the Thiele modulus we know $\eta = 1$ and for very large values of the Thiele modulus we know that $\eta = 3/\Phi = 3/Cd_p$.]

Problem 4-21 **4-22 page 214**

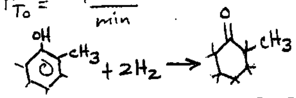
Fragrance Industry: o-creosol, 2-methylcyclohexanone, 2-methylcyclohexanol

1) O order in o-cresol
2) 1^{st} order in H_2
3) $k\Big|_{170°C} = 1.74 \dfrac{mol}{kg_c \text{ min atm}}$

$P_o = 5 atm$

$y_{H_2} = 0.67$, $y_o = 0.33$ } This is stoichiometric

$F_{T_o} = \dfrac{40 \text{ mol}}{\text{min}}$



mole Balance is based on o-cresol (Because problem asks for X_o)

$O + 2H_2 \rightarrow mcH$

Component	initial	change	Final
O	F_{o_i}	$-X_oF_{o_i}$	$F_o = F_{o_i}(1-X_o)$
H_2	$F_{H_{2i}} = 2F_{o_i}$	$-X_o 2F_{o_i}$	$F_{H_2} = 2F_{o_i}(1-X_o)$
mcH	0	$+X_oF_{o_i}$	$F_{mcH} = X_oF_{o_i}$
$F_{T_o} = 3F_{o_i}$			$F_T = 3F_{o_i} - 2X_oF_{o_i}$

$\delta_o = 1-1-2 = -2$

$y_{o_i} = 1/3$

+10

$r_o = -k P_{H_2}$

mole Balance on Packed Bed

$\dfrac{dF_o}{dW} = r_o \qquad -F_{o_i}\dfrac{dX_o}{dW} = -kP_{H_2}$

convert P_{H_2} to $f(X_o)$

$$P_{H_2} = y_{H_2}P = \frac{F_{H_2}}{F_T}P = \frac{F_{o_i}(2-2X_o)}{3F_{o_i}-2X_oF_{o_i}}P = \frac{2P}{3}\left[\frac{(1-X_o)}{(1-\frac{2}{3}X_o)}\right] \Big\} +5$$

a) NEGLECTING Pressure drop $P = P_o$

$$-F_{o_i}\frac{dX_o}{dW} = -kP_o\frac{2}{3}\frac{(1-X_o)}{(1-\frac{2}{3}X_o)} \Rightarrow \int_0^X \frac{(1-\frac{2}{3}X_o)}{(1-X_o)}dX_o = \frac{2kP_o}{3F_{o_i}}\int_0^W dW$$

using Appendix A.2 equation A-7 with $\epsilon = \delta y_{A_o} = -2/3$

$$\int_{X_o=0}^{X_o} \frac{(1-\frac{2}{3}X_o)}{(1-X_o)}dX_o = \left[-(1-\tfrac{2}{3})\ln(1-X) + \tfrac{2}{3}X_o\right]_{X_o=0}^{X_o} = -\frac{1}{3}\ln(1-X_o) + \frac{2}{3}X_o$$

$$= \frac{2}{3}\frac{kP_o}{F_{o_i}}W = -\frac{1}{3}\ln(1-X_o) + \frac{2}{3}X_o$$

+10

NOTE $P = P_o$

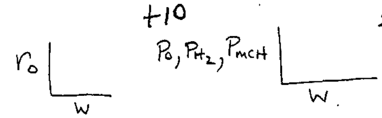
$P_o = y_oP = \dfrac{F_o}{F_T}P_o = P_o\dfrac{(1-X_o)}{(3-2X_o)}$

$2P_o = P_{H_2} = y_{H_2}P_o = \dfrac{F_{H_2}}{F_T}P_o = P_o\dfrac{(1-X_o)}{(3/2-X_o)}$

$P_{mcH} = \dfrac{F_{mcH}}{F_T}P_o = \dfrac{X_o}{(3-2X_o)}P_o$

$r_o = -kP_{H_2} = -kP_o\dfrac{(1-X_o)}{(3/2-X_o)}$

Plot



$$2\frac{\left(1.74\frac{mol\ o}{kg_c \text{ min atm}}\right)(5 atm)W}{\left(40\frac{mol\ T}{min}\right)\left(0.333\frac{mol\ o}{mol\ T}\right)} = -\ln(1-X_o) + 2X_o$$

$$\frac{1.305}{kg}W = -\ln(1-X_o) + 2X_o \Big\} +10$$

Appropriate values of W must be chosen for $X = 0.9999$

$W \leq \dfrac{11.21}{1.305} = 8.59$

Weight $\Rightarrow$ $X = 0.05$ $W = 0.116$

$X = 0.95$, $X = 0.90$: $W/_{0.95} - W/_{0.90} = 3.7515 - 3.144 = 0.6075$

$X_f = 0.95$ Ratio $= \dfrac{0.6075}{0.116} = 5.2$ ← this number will vary since final Conversion was not specified in problem Statement

$X_f = 1.0$ $= \dfrac{\infty}{0.116} = \infty$

Student Handout

Partial Pressure Plots

As before $P_i = y_i P$, but P varies with W

$$P_o = y_o P = P\frac{(1-X_o)}{(3-2X_o)} = \left(\frac{P}{P_0}\right)\frac{P_0(1-X_o)}{(3-2X_o)}$$

$$2P_o = P_{H_2}$$

$$P_{MCH} = \frac{X_o P}{(3-2X_o)}$$

$$-r_o = kP_{H_2} = 2kP\frac{(1-X_o)}{(3-2X_o)} = kP\frac{(1-X_o)}{(3/2-X_o)}$$

part C

Alternative 1: increase D_p to reduce ΔP

Alternative 2: shorter Reactor with $2D_{pipe\,old} = D_{pipe\,New}$

$$A_c\big|_{old} = \frac{\pi D_{pipe\,old}^2}{4}$$

$$A_c\big|_{New} = \frac{\pi 4 D_{pipe\,old}^2}{4}$$

$$A_{c_N} = 4A_{c\,old}$$

$$\frac{2}{3}\frac{k P_0}{F_{0i}} = \text{constant}$$

what changes?

$$\beta_0 = \frac{G(1-\phi)}{\rho_0 D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]$$

$$\alpha = \frac{2\beta_0}{A_c \rho_c (1-\phi) P_0}$$

$$\alpha = \left[\frac{2G\cancel{(1-\phi)}}{\rho_0 \phi^3 \rho_c P_0 \cancel{(1-\phi)}}\right]\left(\frac{1}{D_p A_c}\right)\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]$$

G – constant $\therefore G = \rho_0 v_0$

P_0 "

ρ_c "

$\therefore$ Increasing D_p $\underbrace{\text{has the same effect as}}_{\text{Both Reduce } \alpha}$ increasing A_c !

10 pts

$\hookrightarrow X\uparrow$

$\hookrightarrow P/P_0\uparrow$

1) – Problems W ≥ 5

0.01	5	0.885	– 0.23
0.001	5 –	0.885	0.0123
0.00005	5 –		

failure

$\alpha = 0.17$
$\alpha = 0.1$
$\alpha = 0.15$
$\alpha = 0.12$
$\alpha = 0.05$

C4P23A

make graph & copy

Part b 4-22

Account for pressure drop given $\alpha = 0.34\ \text{kg}^{-1}$

start with $\dfrac{dP}{dL} = -\dfrac{\rho_0}{\rho}\beta_0$

mass balance

$A_c \rho v = \rho_0 v_0 A_c$

$T = T_0$

$$\frac{\rho}{\rho_0} = \frac{v_0 A_c}{v A_c} = \frac{\varphi_0}{\varphi} = \frac{P F_{T_0} \cancel{R T_0}}{P_0 F_T \cancel{RT}}$$

$$W = L A_c(1-\phi)\rho_c$$

$$dW = dL\, A_c(1-\phi)\rho_c$$

$$\frac{1}{dL} = \frac{A(1-\phi)\rho_c}{dW}$$

$$\frac{\rho}{\rho_0} = \frac{P}{P_0}\frac{3\cancel{F_{oi}}}{\cancel{F_{oi}}(3-2X_o)}$$

$$\frac{\rho}{\rho_0} = \frac{P}{P_0}\frac{1}{(1-\frac{2}{3}X_o)}$$

$$\frac{dP}{dW} = -\frac{P_0}{P}\frac{(1-\frac{2}{3}X_o)}{A\rho_c(1-\phi)}\beta_0$$

from book $\alpha = 2\beta_0/(A_c\rho_c(1-\phi)P_0)$

Divide both sides by P_0

(1) $$\frac{d(P/P_0)}{dW} = -\frac{P_0}{P}\left(1-\tfrac{2}{3}X_o\right)\frac{\alpha}{2}$$

$$\frac{dF_o}{dW} = r_o$$

(2) $$\frac{dX_o}{dW} = k\frac{2P}{3}\left[\frac{(1-X_o)}{(1-\frac{2}{3}X_o)}\right]\frac{1}{F_{oi}}$$

```
Problem 4-22  Examine pressure drop effect on reaction rate
d(PP0)/d(W)=-(1-2*X/3)*alpha/2/PP0
d(X)/d(W)=1.74*2/3*PP0*5*(1-X)/(1-2/3*X)/(40*.33)
alpha=0.34
W(0)=0
PP0(0)=1
X(0)=0
W(f)=5
```