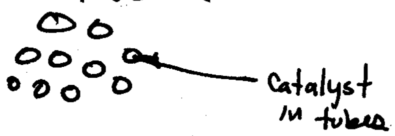
Packed Bed Reactors

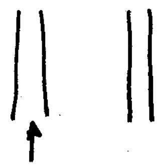
1) majority of commercial gas-phase catalytic processes

2) Exceptions – fluidized bed
   - continuously regenerate catalyst – cracking
   - improve heat removal – syn {acrylonitrile, ethylenedichloride}
     naphthalene oxidation to phthalic anhydride

3) Fixed bed reactors
   - simple technology (adiabatic reactors)
   - exothermic rxns, endothermic rxns } need multibed reactors

   a) multitubular FBR





2.5cm, ID
20,000 tubes

   b) multibed reactors 

Scale-up
1) empirical (semi-) lab – pilot .... commercial
2) fundamental

Need modeling

problems: complex hydrodynamics
lack of detailed & accurate kinetics

procedure – find kinetics without diffusional limitations
catalyst deactivation

PFR

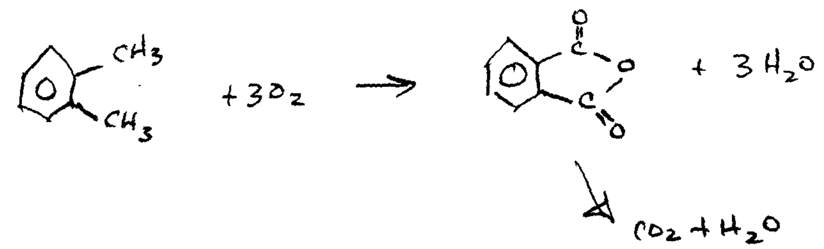
(1) Show transparency — Chemical Engineering Science (1985)

<u>Phthalic Anhydride manufacture</u> $\rightarrow$ exothermic

Vertical shell & tube heat exchanger

catalyst in tubes (solid spheres, rings etc.

molten salt in shell side { Na-K & nitrates



$\Delta H_{rxn} = -265 \frac{kcal}{gmol}$

45,000 metric ton/yr $\rightarrow$ ~ 20,000 tubes with ID ~ 2.5 cm

tube length 3.65 m

Previous work — keep mixture below flammable limits

current reactors — working above the flammability limits }

V_2O_5 catalyst with TiO_2 + promotors } 10 wt%

non-porous carborundum }

$d_p = 6\,mm$

$6/26 = \frac{d_P}{ID_{tube}} = 0.23$

$\rho_c \cong 1{,}780 \frac{kg_c}{m^3_{cat}}$

assume $\phi = 0.45$

Perry's Figure 5-70

Cylindrical Rings — $\phi = 0.47$

Spheres — $\phi \cong 0.45$

Raschig Ring — $\phi = 0.6$

$\rho_{bulk} = \rho_c(1-\phi)$

$\frac{kg_{cat}}{m^3_{cat}} \quad \frac{m^3_{cat}}{m^3_{Bed}}$

$\rho_{bulk} = 980\, kg/m^3_{Bed}$

(m^3_{cat}/m^3_{Bed})

PFR & Pressure Drop

"Fixed" Bed
"Packed" Beds } need to consider pressure drop in calculations of X.

(Read Section 4.3 to see the effect of gas expansion on conversion).

Rase H.F., Fixed-Bed Reactor Design and Diagnostics, Gas Phase Reactions, Butterworths 1990 p 167

High Range: once through Reactors; nonadiabatic reactors with high velocities provide heat transfer efficiency for controlling hot spots.

I. $0.01 P_{T} \lesssim \Delta P \lesssim 0.10 P_T$

low Range: Recycle or large flows of gas or multiple adiabatic beds

Flow through an empty tube

laminar flow (Hagen-Poiseuille): $v = \frac{R^2}{8\mu}\left(-\frac{\Delta P}{L}\right)$

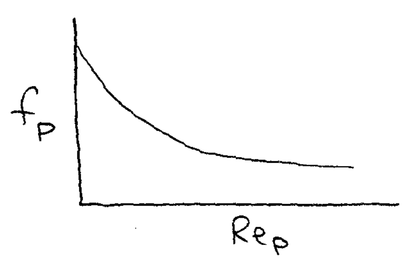
or $\Delta P = -\frac{8 v \mu L}{R^2}$

turbulent flow:

$$\frac{\Delta P}{L} = \underbrace{\left(\frac{2\rho f}{D}\right)}_{C_v} v_\infty^2 \qquad \text{where } v_\infty = \frac{Q}{A}$$

superficial velocity

Flow through a packed Bed: Ergun Equation



3 eqns

$$\frac{dP}{dL} = -\frac{f_p \rho}{D_p}\left[\frac{(1-\phi)}{\phi^3}\right] v_\infty^2 \qquad \text{and} \qquad f_p = \frac{150}{Re_p} + 1.75$$

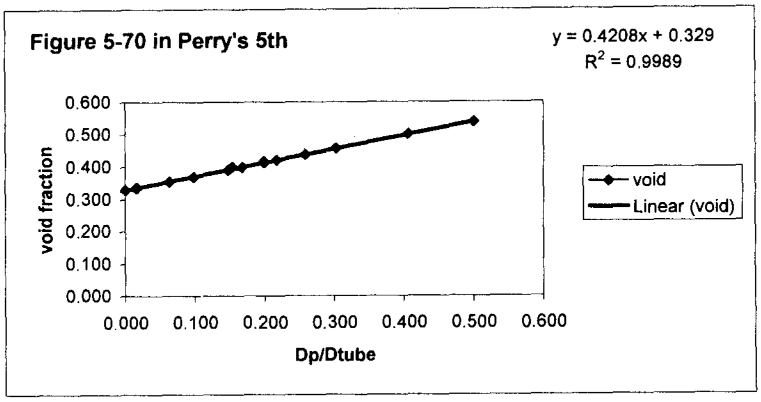
$$Re_p = \frac{\rho D_p}{\mu}\left[\frac{v_\infty}{1-\phi}\right]$$

where ϕ - void fraction $= \frac{\text{void volume (gas)}}{\text{Reactor Volume}}$

Void Fraction Curve for spheres
Taken from Perry's 5th Edition
Figure 5-70

Scale x	0.003671
Scale y	0.003636

Dp/Dtube x	void y	Dp/Dtube	void
0	7.86	0.000	0.329
4.21	9.56	0.015	0.335
4.71	9.86	0.017	0.336
17.21	14.86	0.063	0.354
26.71	18.96	0.098	0.369
40.21	24.86	0.148	0.390
41.71	27.36	0.153	0.399
45.71	27.16	0.168	0.399
54.21	31.86	0.199	0.416
54.21	30.86	0.199	0.412
59.11	**32.96**	**0.217**	**0.420**
70.31	37.86	0.258	0.438
82.51	42.86	0.303	0.456
110.71	55.21	0.406	0.501
136.2	65.36	0.500	0.538



linear fit to spherical data
y = 0.4208x + 0.329

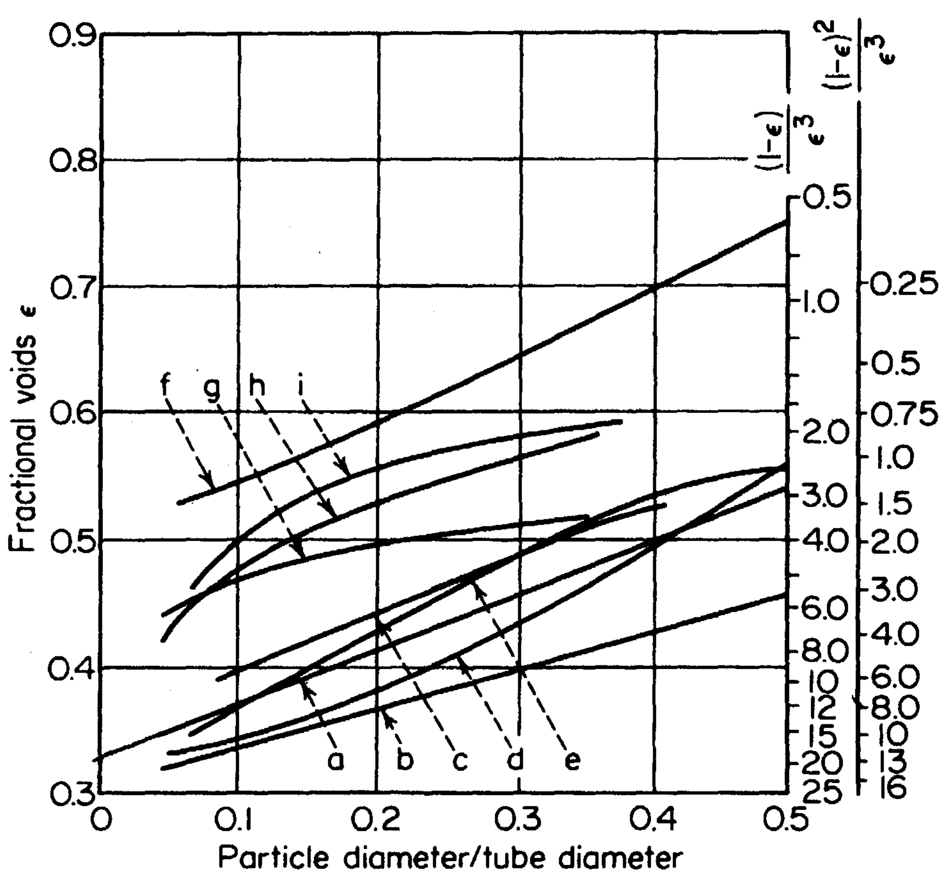


Fig. 5-70. Voidage in packed beds. Spherical: *a*, smooth, uniform; *b*, smooth, mixed; *c*, clay. Cylindrical: *d*, smooth, uniform; *e*, alundum, uniform; *f*, clay Raschig rings. Granules: *g*, fused magnetite (synthetic ammonia catalyst); *h*, fused alundum; *i*, Aloxite. (*Leva, "Fluidization," p. 54, McGraw-Hill, New York, 1959.*)

Fogler Ergun

$$\frac{dP}{dz} = -\frac{G}{\rho D_p}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_p} + 1.75\,\underbrace{G}_{\frac{kg}{m^2 s}}\right] \qquad 4\text{-}22$$

BSL 6.4-13

$$\left(-\frac{dP}{dL}\right)\frac{\rho}{G_0^2} D_p \frac{\varepsilon^3}{1-\varepsilon} = 150\left(\frac{1-\varepsilon}{D_p G_0/\mu}\right) + 1.75 \qquad 6.4\text{-}13$$

$$\frac{dP}{dL} = \frac{G_0^2}{\rho D_p}\left(\frac{1-\varepsilon}{\varepsilon^3}\right)\left[150\frac{(1-\varepsilon)}{D_p G_0/\mu} + 1.75\right]$$

$$G_0 = \frac{kg}{m^2 s}$$

$$= \frac{G_0}{\rho D_p}\left(\frac{1-\varepsilon}{\varepsilon^3}\right)\left[\frac{150(1-\varepsilon)}{D_p/\mu} + 1.75 G_0\right]$$

Geankoplis eqn 3.1-20

$$\frac{\Delta P}{\Delta L} = \frac{150\mu v'}{D_p^2}\frac{(1-\varepsilon)^2}{\varepsilon^3} + \frac{1.75(v')^2\rho}{D_p}\frac{1-\varepsilon}{\varepsilon^3}$$

$$= \frac{v'}{D_p}\frac{1-\varepsilon}{\varepsilon^3}\left[\frac{150\mu(1-\varepsilon)}{D_p} + 1.75 v'\rho\right]$$

$$\underbrace{v'}_{\text{superficial}} = \varepsilon v \qquad v' A_c \rho = G A_c$$

$$v' = G/\rho$$

$$\frac{\Delta P}{\Delta L} = \frac{G}{\rho D_p}\frac{1-\varepsilon}{\varepsilon^3}\left[\frac{150\mu(1-\varepsilon)}{D_p} + 1.75\frac{G\cancel{\rho}}{\cancel{\rho}}\right]$$

Froment & Bischoff

$$-\frac{dP}{dz} = f \, \frac{\rho u_s^2}{d_p} \qquad 11.5.1\text{-}3$$

$$f = \frac{1-\varepsilon}{\varepsilon^3}\left[a + \frac{b(1-\varepsilon)}{Re_p}\right] \qquad 11.5.1\text{-}13$$

$$-\frac{dP}{dz} = \frac{1-\varepsilon}{\varepsilon^3}\,\frac{\rho u_s^2}{d_p}\left[a + \frac{b(1-\varepsilon)}{Re_p}\right]$$

$$\rho u_s = G$$

$$= \frac{1-\varepsilon}{\varepsilon^3}\,\frac{G^2}{\rho\, d_p}\left[a + \frac{b(1-\varepsilon)}{Re_p}\right]$$

$$= \frac{1-\varepsilon}{\varepsilon^3}\,\frac{G}{\rho D_p}\left[Ga + \frac{Gb(1-\varepsilon)}{Re_p}\right]$$

$$Re_p = \frac{D_p \rho u_s}{\mu}$$

$$= \frac{1-\varepsilon}{\varepsilon^3}\,\frac{G}{\rho D_p}\left[Ga + \frac{\cancel{G}\, b\,(1-\varepsilon)\mu}{D_p \cancel{\rho u_s}}\right]$$

where $a = 1.75 \quad b = 150$

Tallmadge (1970) $\quad b = 4.2\, Re^{5/6}$

$$\frac{1-\varepsilon}{\varepsilon^3}\,\frac{G}{\rho D_p}\left[Ga + \frac{G(1-\varepsilon)\, 4.2\, Re^{5/6}}{Re_p}\right]$$

$$\left[Ga + \frac{G(1-\varepsilon)}{Re_p^{1/6}}\, 4.2\right]$$

Froment & Bischoff[3]

Tallmadge (1970) cont.

$$= \frac{1-\varepsilon}{\varepsilon^3} \frac{G}{\rho D_p} \left[G_a + \frac{G(1-\varepsilon) 4.2 \mu^{1/6}}{(D_p \rho u_s)^{1/6}} \right]$$

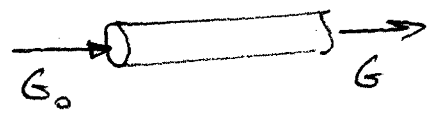
Good correlation of ϕ is given in Perry's

plug in f_p & Re_p

$$\frac{dP}{dz} = -\frac{\rho v_\infty^2}{D_p}\frac{(1-\phi)}{\phi^3}\left[\frac{150(1-\phi)\mu}{D_p\,\rho\, v_\infty} + 1.75\right]$$

this form is not very easy to use

So convert to a form using a mass balance



$G\ [=]\ \frac{kg}{m^2\,s}$ ← total cross sectional area

$$G = \rho\, v_\infty A = \rho\left[\frac{Q}{A}\right]A$$

$\frac{Q}{A}$ ← v_∞

3rd ed
eqn 4-22

eqn 4-23
$$\left\{\ \frac{dP}{dz} = -\frac{1}{\rho}\underbrace{\frac{G}{D_p}\frac{(1-\phi)}{\phi^3}}_{}\underbrace{\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]}_{\text{constant with } z}\left(\frac{\rho_o}{\rho_o}\right)\right. \leftarrow \beta_o$$

↑ variable density – T or # moles

let $\frac{dP}{dz} = \frac{-1}{\rho}\left[\rho_o \beta_o\right]$ and β_o = equation ~~4-31~~ 4-25 3rd ed.

Variable Density: (continued

$$\frac{\rho_0}{\rho} = \frac{P_0}{P}\frac{T}{T_0}\frac{F_T}{F_{T_0}} = \frac{P_0}{P}\frac{T}{T_0}\left[1 + \delta \underbrace{\frac{F_{A0}}{F_{T_0}}}_{y_{A0}\text{ - mole fraction}} X_A\right]$$

$\underline{\underline{\text{variable density i)}}}$ if $y_{A_0} \to 0$ dilute gas or $\delta = 0$ or small $\Big\}$ & $\underline{\underline{T = T_0}}$

$$\frac{\rho_0}{\rho} = \frac{P_0}{P}\frac{T}{T_0}$$

$$\frac{dP}{dz} = -\beta_0\left[\frac{P_0}{P}\frac{T}{T_0}(1+0)\right]$$

$$\int P\,dP = -\beta_0 P_0 \frac{T}{T_0}\int dz$$

$$\left.\frac{P^2}{2}\right|_{P_0}^{P} = -\left[\beta_0 P_0 \frac{T}{T_0}\right](z) \qquad \frac{P^2}{2} - \frac{P_0^2}{2} = -\beta_0 P_0 \frac{T}{T_0} z$$

$$P = \left[P_0^2 - 2\beta_0 P_0 \frac{T}{T_0} z\right]^{1/2}$$

variable density ii)) $T \neq T_0$ and $y_{A_0} \neq 0$ $\delta_A \neq 0$

<u>Numerical integration</u>

Now we need a relation for $\frac{\rho_o}{\rho}$

$$\frac{dP}{dz} = -\beta_o\left[\frac{\rho_o}{\rho}\right]$$ ← I will give this equation on the exam.

I assume $\rho \simeq \bar{\rho}$

$$\frac{dP}{dz} = -\underbrace{\frac{\rho_o}{\bar{\rho}}}_{\text{constant}}\beta_o \quad \text{integrate} \quad P = P_o - \underbrace{\left[\frac{\rho_o}{\bar{\rho}}\beta_o\right]}_{\text{Constant}} z$$

II Variable Density

find a relation for $\frac{\rho_o}{\rho}$

mass balance: $\rho_o v_{\infty_o} = \rho v_\infty$

$G_o = G$

$$\frac{\rho_o}{\rho} = \frac{v_\infty}{v_{\infty_o}} = \frac{\Phi/A}{\Phi_o/A}$$

$$\frac{P\Phi}{P_o\Phi_o} = \frac{F_T RT}{F_{T_o} RT_o}$$

$$\frac{\Phi}{\Phi_o} = \frac{P_o}{P}\frac{F_T}{F_{T_o}}\frac{T}{T_o}$$

$$\therefore \frac{\rho_o}{\rho} = \frac{P_o}{P}\frac{F_T}{F_{T_o}}\frac{T}{T_o}$$