Fluid-fluid Reaction: Kinetics and Reactor Design

Book: *Chemical Reaction Engineering*, O. Levenspiel, (Chapter 23 and 24), 3rd Edition, Wiley and Sons

Fluid-fluid reactor design

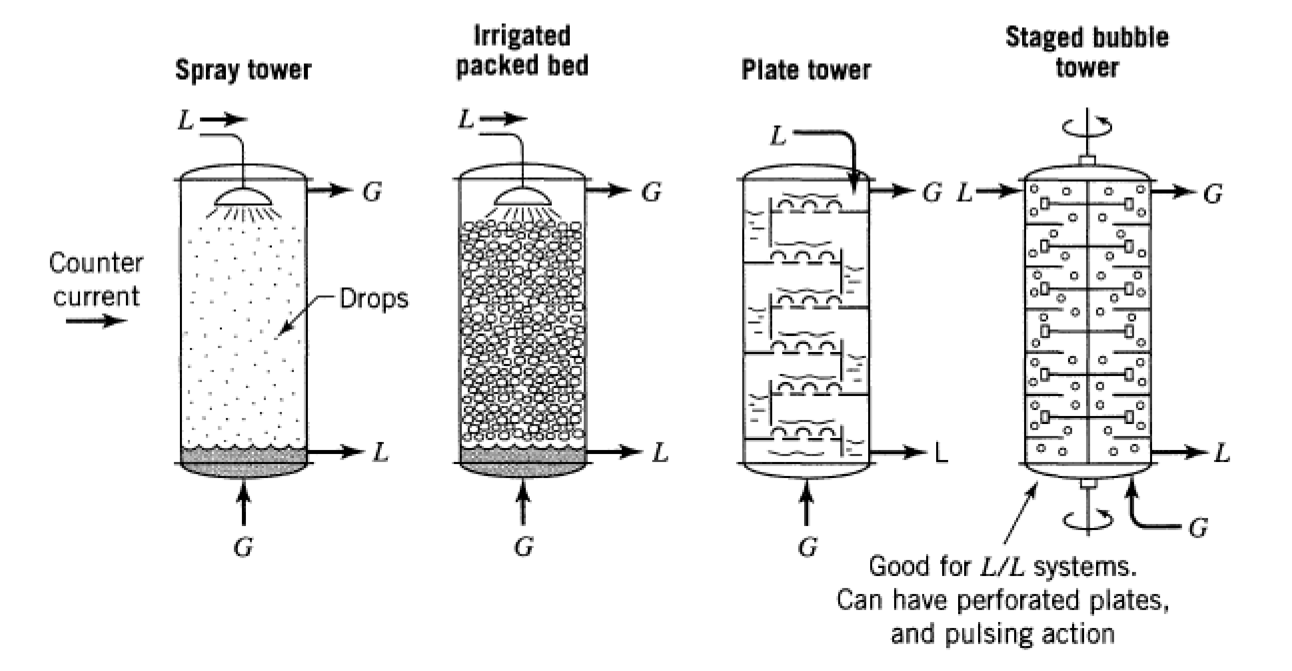
- It is essential to first choose the right kind of contactor and then find the size needed
- Contactors are mainly of two kinds –

(a) Towers – spray tower,

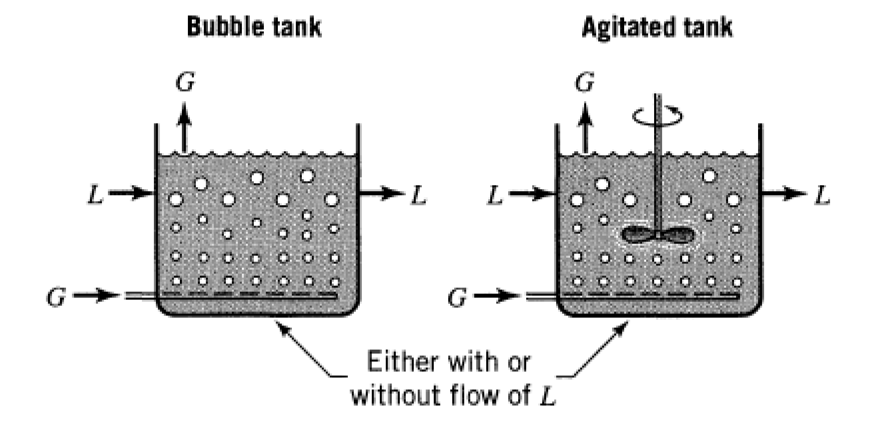
– irrigated packed beds,

– plate tower,

– staged bubble tower



(b) Tanks – Bubble tank, Agitated tank



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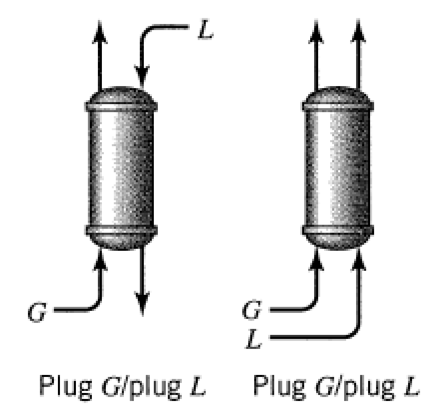
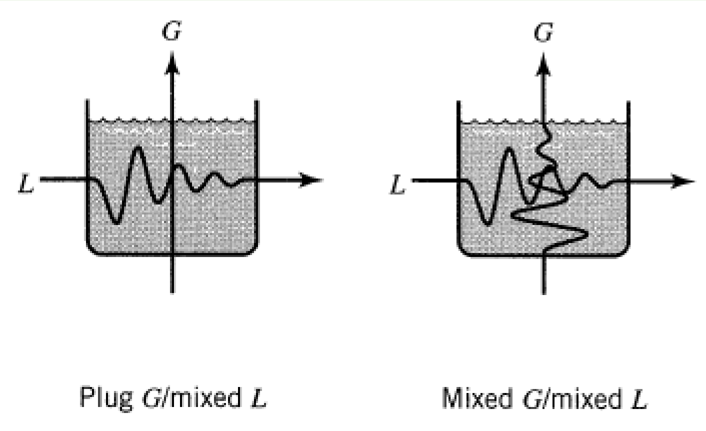
Factors to consider in selecting a contactor

(1) **Contacting pattern:**

- Towers approximate – plug G/plug L
- Bubble tanks approximate – plug G/mixed L
- Agitated tanks approximate – mixed G/mixed L
- Towers have the largest mass transfer driving force while agitated tanks have the smallest driving force





(2) $\boldsymbol{k_g}$ **and** $\boldsymbol{k_L}$:

- For liquid droplets in gas, k_g is high and k_L is low
- For gas bubbles rising in liquid, k_g is low and k_L is high

(3) **Flow rates:**

- Packed beds work best with relative flow rates of about $F_l/F_g \approx 1$ at 1 bar
- Other contactors work over wide ranges of F_l/F_g values

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(4) **If resistance is in the gas and/or liquid films:**

- Large interfacial area 'a' is desired – use agitated contactors and most columns
- If liquid film dominates – do not use spray contactors
- If gas film dominates – do not use bubble contactors

(5) **If the resistance is in the main body:**

- Large f_l $(= {}^{V_l}/_{V_r})$ is desired – use tank contactor, avoid towers

(6) **Solubility:**

- For very soluble gases (small values of Henry's law constant, H_A) gas film controls – do not use bubble contactors
- For gases of low solubility (large values of Henry's law constant, H_A) liquid film controls – do not use spray towers

(7) **Reaction lowers the resistance of liquid films:**

- For absorption of highly soluble gases, chemical reaction is not helpful
- For absorption of slightly soluble gases, chemical reaction is helpful and speeds up the rate

Processes involving straight mass transfer

First, systems that involve only the absorption of A by the liquid is considered

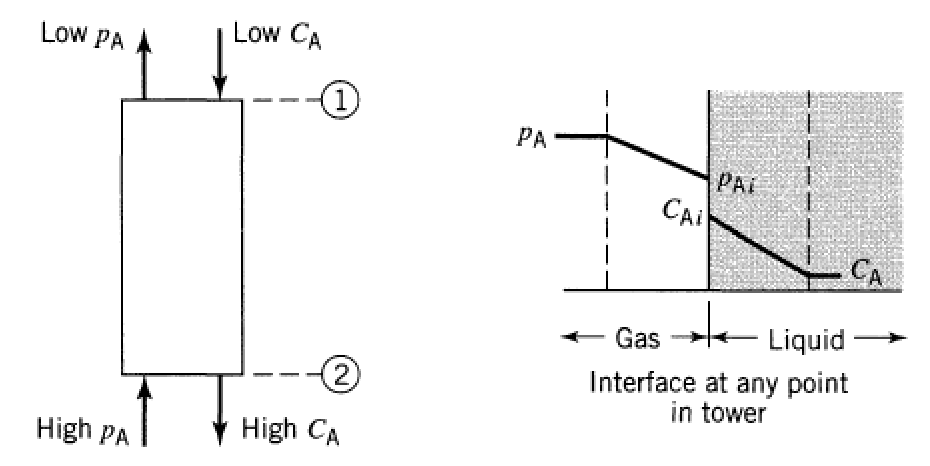
$$A(gas) \rightarrow A(liquid)$$

(1) Plug flow gas/Plug flow liquid – counter current flow in a tower

- To develop the performance equation, the rate equation is combined with the material balance
- Thus for steady state, counter current operations, and a differential element of volume,

$$(A\ lost\ by\ gas) = (A\ gained\ by\ liquid) = (-r_A''')dV_r$$

$$F_g dY_A = F_l dX_A = (-r_A''')dV_r$$



$F_g = \frac{F_g' p_U}{\pi}$ = upward molar flow rate of inerts in the gas (mol/s)

F_g' = molar flow rate all the gas (mol/s)

p_U = partial pressure of carrier or inert compound

$\pi = p_A + p_B + \ldots\ldots + p_U$ = total pressure

$F_l = \frac{F_l' C_U}{C_T}$ = downward molar flow rate of inerts in the liquid (mol/s)

F_l' = molar flow rate all the liquid (mol/s)

C_U = concentration of carrier or inert compound in liquid

$C_T = C_A + C_B + \ldots\ldots + C_U$ = total concentration

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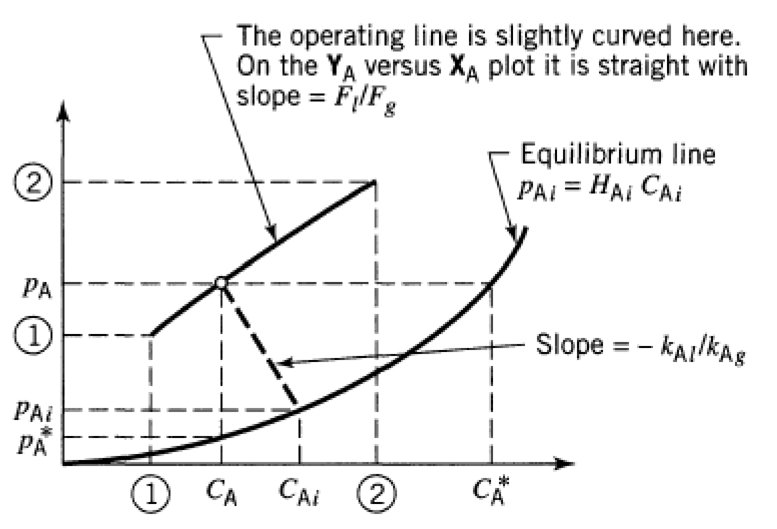
$$dY_A = d\left(\frac{p_A}{p_U}\right) = \frac{p_U dp_A - p_A dp_U}{{p_U}^2} \quad \text{and} \quad dX_A = d\left(\frac{C_A}{C_U}\right) = \frac{C_U dC_A - C_A dpC_U}{{C_U}^2}$$

and, $dY_A = \frac{\pi dp_A}{(\pi - p_A)^2}$ and $dX_A = \frac{C_T dC_A}{(C_T - C_A)^2}$



Now, $(-r_A''') = a(-r_A'') = k_{Ag}a(p_A - p_{Ai}) = k_{AL}a(C_{Ai} - C_A)$

Integrating for the whole tower,

$$V_r = \frac{F_g}{a}\int_{Y_{A1}}^{Y_{A2}} \frac{dY_A}{(-r_A'')} = \frac{F_l}{a}\int_{X_{A1}}^{X_{A2}} \frac{dX_A}{(-r_A'')}$$

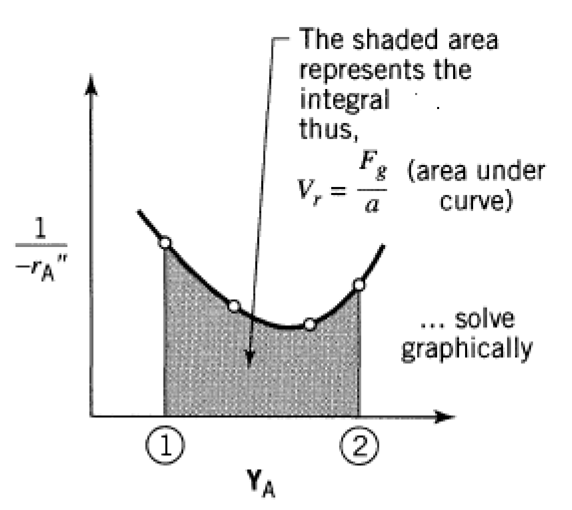
Replacing dY_A by dp_A

$$V_r = F_g\pi\int_{p_{A1}}^{p_{A2}} \frac{dp_A}{(\pi - p_A)^2 k_{Ag}a(p_A - p_{Ai})}$$

$$V_r = \int_{p_{A1}}^{p_{A2}} \frac{F_g' dp_A}{k_{Ag}a(\pi - p_A)(p_A - p_{Ai})} \qquad F_g' = \frac{F_g\pi}{p_U} = \frac{F_g\pi}{(\pi - p_A)}$$

$$V_r = F_l C_T\int_{C_{A1}}^{C_{A2}} \frac{dC_A}{(C_T - C_A)^2 k_{AL}a(C_{Ai} - C_A)}$$

$$V_r = \int_{C_{A1}}^{C_{A2}} \frac{F_l' dC_A}{k_{AL}a(C_T - C_A)(C_{Ai} - C_A)} \qquad F_l' = \frac{F_l C_T}{C_U} = \frac{F_l C_T}{(C_T - C_A)}$$



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For dilute solutions, $C_A \ll C_T$ and $p_A \ll \pi$

So, $F_g' \cong F_g$ and $F_l' \cong F_l$

Hence, the material balance becomes, $\frac{F_g}{\pi} dp_A = \frac{F_l}{C_T} dC_A = (-r_A''')dV_r$

For any two points in the absorber, $p_{A_2} - p_{A_1} = \frac{F_l \pi}{F_g C_T}\left(C_{A_2} - C_{A_1}\right)$

Now rate reduces to, $(-r_A''') = a(-r_A'') = \left(\frac{1}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{AL}a}}\right)(p_A - p_A^*)$

$$K_{Ag}a(p_A - p_A^*) = K_{AL}a(C_A^* - C_A)$$

Thus,

$$V_r = hA_{cs} = \frac{F_g}{\pi}\int_{p_{A1}}^{p_{A2}} \frac{dp_A}{(-r_A''')} = \frac{F_g}{\pi K_{Ag}a}\int_{p_{A1}}^{p_{A2}} \frac{dp_A}{(p_A - p_A^*)}$$

where $\frac{1}{K_{Ag}} = \frac{1}{k_{Ag}} + \frac{H_A}{k_{AL}}$ and $p_A^* = H_A C_A$

or,

$$V_r = hA_{cs} = \frac{F_l}{C_T}\int_{C_{A1}}^{C_{A2}} \frac{dC_A}{(-r_A''')} = \frac{F_l}{C_T K_{AL}a}\int_{C_{A1}}^{C_{A2}} \frac{dC_A}{(C_A^* - C_A)}$$

where $\frac{1}{H_A K_{AL}} = \frac{1}{k_{Ag}} + \frac{1}{k_{AL}}$ and $C_A^* = {p_A}/{H_A}$

Example

The concentration of undesirable impurity in air (at 1 bar = 10^5 Pa) is to be reduced from 0.1% (or 100 Pa) to 0.02% (or 20 kPa) by absorption in pure water

Find the height of the tower required for counter current operations

For the packing,

$k_{Ag}a$ = 0.32 mol/h.m^3. Pa

$k_{AL}a$ = 0.1 h^{-1}

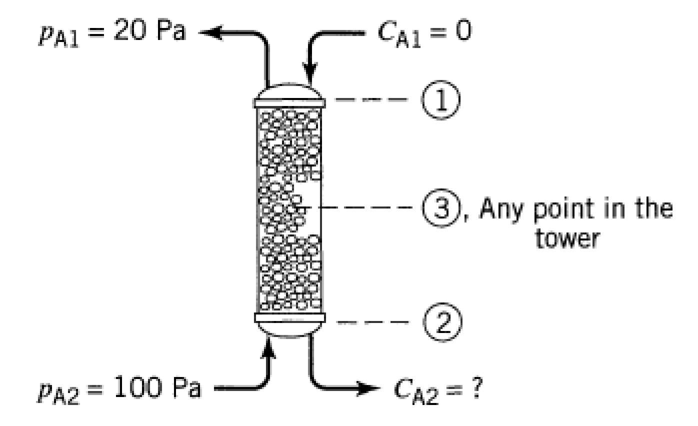
H_A = 12.5 Pa.m^3 /mol

$\frac{F_g}{A_{cs}}$ = 1 x 10^5 mol/h.m^2

$\frac{F_l}{A_{cs}}$ = 7 x 10^5 mol/h.m^2

C_T = 56000 mol/m^3

The material balance is first solved as shown below,



At any point in the absorption tower, $p_A - p_{A_1} = \frac{F_l \pi}{F_g C_T}(C_A - C_{A_1})$

$$p_A - 20 = \frac{7\times10^5\times10^5}{1\times10^5\times 56000}(C_A - 0)$$

$$p_A - 20 = 12.5\, C_A$$

$$C_A = 0.08 p_A - 1.6$$

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The value of C_{A_2} can be calculated from $C_{A_2} = 0.08p_{A_2} - 1.6 = 0.08 \times 100 - 1.6 = 6.4$ mol/m³

The tower height is then determined in the following way,

$$h = \frac{V_r}{A_{cs}} = \frac{\frac{F_g}{A_{cs}}}{\pi K_{Ag} a} \int_{p_{A1}}^{p_{A2}} \frac{dp_A}{(p_A - p_A^*)}$$

$$\frac{1}{K_{Ag}a} = \frac{1}{k_{Ag}a} + \frac{H_A}{k_{AL}a} = \frac{1}{0.32} + \frac{12.5}{0.1} = 128.125 \qquad \Rightarrow \qquad K_{Ag}a = 0.007805 \text{ mol/h.m}^3\text{.Pa}$$

Now,

$$\begin{aligned} p_A - p_A^* &= p_A - H_A\, C_A \\ &= p_A - H_A(0.08p_A - 1.6) = p_A - 12.5(0.08p_A - 1.6) \\ &= p_A - p_A + 20 = 20 \end{aligned}$$

$$h = \frac{V_r}{A_{cs}} = \frac{1 \times 10^5}{10^5 \times 0.007805} \int_{20}^{100} \frac{dp_A}{20}$$

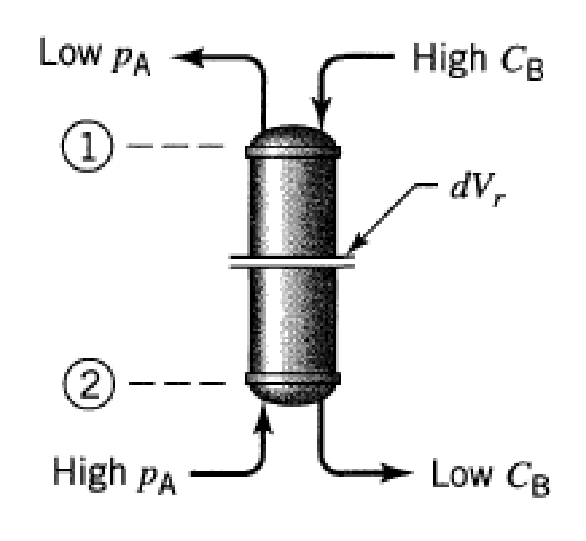
$$h = 128.125\left(\frac{100-20}{20}\right) = 512.5 \text{ m}$$

Mass transfer + Not very Slow Reaction

The reaction $A(g \to l) + bB(l) \to products$ occurs at a rate fast enough so " no unreacted A enters the main body of the liquid"

Hatta No is not much smaller than unity; reaction is in gas or liquid film

(2) Plug flow gas/Plug flow liquid – Mass Transfer + Reaction in counter-current tower



For a differential slice of absorber - reactor

$$(A\ lost\ by\ gas) = \frac{1}{b}(B\ lost\ by\ liquid) = (Disappearance\ of\ A\ by\ reaction)$$

$$F_g dY_A = \frac{F_l dX_B}{b} = (-r_A''')dV_r$$

or, $$\frac{F_g}{\pi} dp_A = \frac{F_l}{bC_T} dC_B = (-r_A'')a dV_r$$ $\because\ p_U = \pi$ and $C_U = C_T$

Therefore, $$V_r = F_g \int_{Y_{A1}}^{Y_{A2}} \frac{dY_A}{(-r_A'')a} = \frac{F_l}{b} \int_{X_{B2}}^{X_{B1}} \frac{dX_B}{(-r_A'')a}$$ with $F_g\left(Y_{A_2} - Y_{A_1}\right) = \frac{F_l}{b}\left(X_{B_1} - X_{B_2}\right)$

For dilute systems,

$$V_r = \frac{F_g}{\pi} \int_{p_{A1}}^{p_{A2}} \frac{dp_A}{(-r_A'')a} = \frac{F_l}{bC_T} \int_{C_{B2}}^{C_{B1}} \frac{dC_B}{(-r_A'')a}$$ with $$\frac{F_g}{\pi}\left(p_{A_2} - p_{A_1}\right) = \frac{F_l}{bC_T}\left(C_{B_1} - C_{B_2}\right)$$

$$V_r = \frac{F_g}{\pi}\int_{p_{A1}}^{p_{A2}} \frac{dp_A}{(-r_A'')a} = \frac{F_l}{bC_T}\int_{C_{B2}}^{C_{B1}} \frac{dC_B}{(-r_A'')a}$$

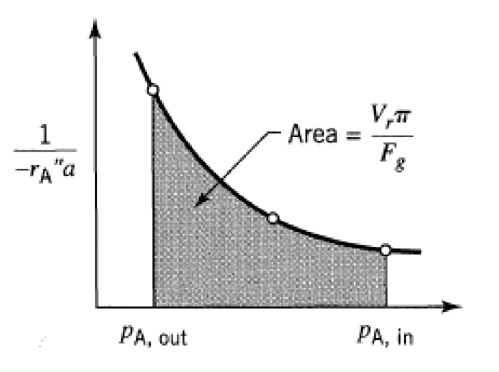
with $\frac{F_g}{\pi}(p_{A_2} - p_{A_1}) = \frac{F_l}{bC_T}(C_{B_1} - C_{B_2})$

To solve for V_r

- Few p_A values are chosen, usually p_{A_1}, p_{A_2} and one intermediate value and corresponding C_B is evaluated for each p_A
- Rates are evaluated for each point

$$(-r_A'')a = \frac{p_A}{\frac{1}{k_{Ag}a} + \frac{H_A}{k_{AL}aE} + \frac{H_A}{kC_Bf_L}}$$

- The values are plotted and integrated graphically



(3) Plug flow gas/Plug flow liquid – Mass Transfer + Reaction in co-current tower

Here the equations developed for counter-current can be used with a few changes

F_l to $-F_l$ (for up flow of both streams) and F_g to $-F_g$ (for downflow of both streams)

C_B values are evaluated for each p_A; rest of the procedure is the same