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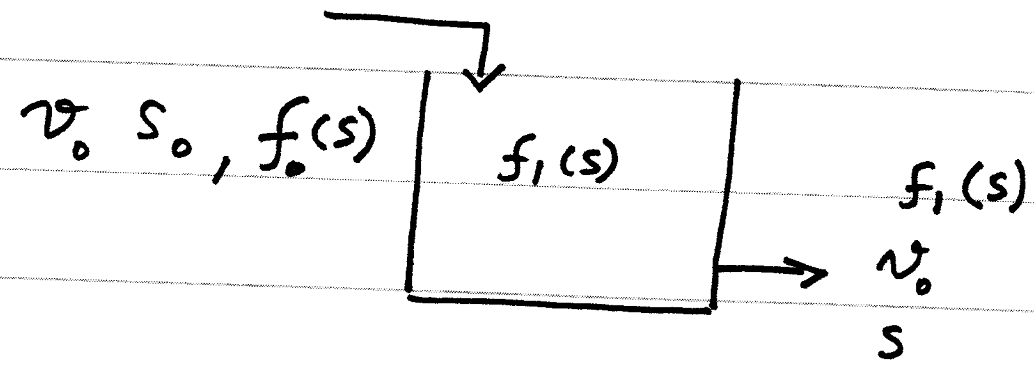
Population Balance Modelling

Material Balance on a CSTR.



$$v_0 \bar{S}_0 - v_0 \bar{S} + \bar{r} V = \frac{\partial V \bar{S}}{\partial t} \qquad - \quad (1).$$

$$\bar{S}_0 = \int s f_0(s)\, ds \quad ; \quad \bar{S} = \int s f_1(s)\, ds \; ; \quad \bar{r} = \int r f_1(s)\, ds$$

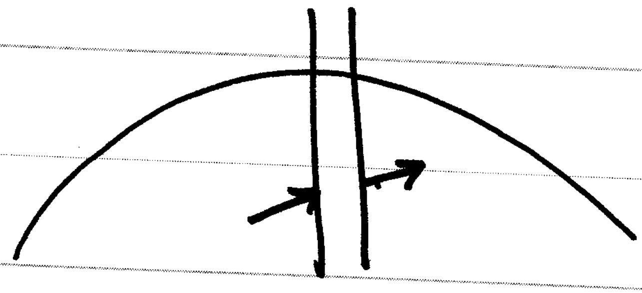
$$v_0 \int s f_0(s)\, ds - v_0 \int s f_1(s)\, ds + \int \underbrace{\overset{\mathrm{I}}{r}\, f_1 \overset{\mathrm{II}}{(s)}}\, ds \cdot V = \frac{\partial}{\partial t}\left(V \int s f_1 ds\right.$$

$$v_0 \int s_0 f_0(s)\,ds - v_0 \int s f_1(s)\,ds + \cancel{\left[r V f_1(s) s \right]} - \int s \frac{\partial}{\partial s}\cdot(r f_1)\,ds . V$$

$$= \frac{\partial}{\partial t}\cdot \left[V \int s f_1\,ds \right].$$

$$v_0 \int s f_0\,ds - v_0 \int s f_1\,ds - \int s \frac{V \partial}{\partial s}\cdot(r f_1)\,ds = \frac{\partial}{\partial t}\cdot \int s f_1\,ds . V \quad \text{— (2)}$$

$$v_0 f_0 - v_0 f_1 - \frac{\partial}{\partial s}\cdot(r f_1 V) = \frac{\partial}{\partial t}(f_1 V) \quad \text{— (3)}$$



$$1/p - 0/p + G = Acc$$

$$\frac{d t}{ds} \quad v_0 f_0(s)ds - v_0 f_1(s)ds + \Big[W f_1(s) r_1(s)\Big]_s - \Big[W f_1(s) r_1(s)\Big]_{s+ds}$$

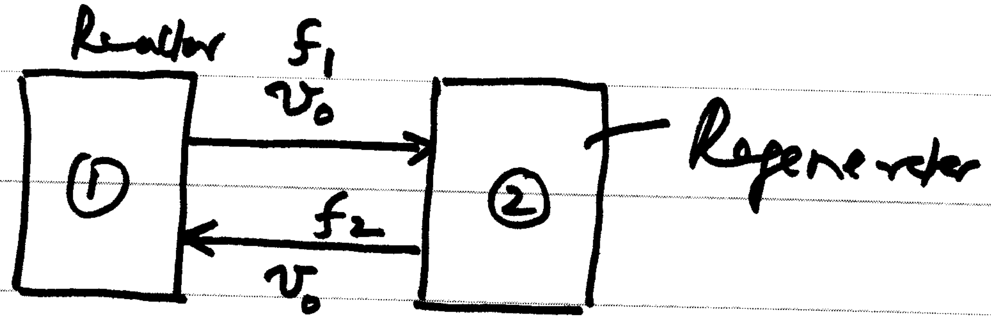
$$+ B(s)\delta(s-0)ds - D(s)ds.$$

$$= \frac{\partial}{\partial t}\cdot(W f_1 \cancel{ds}).$$

$$v_0 f_0 - v_0 f_1 - \frac{\partial}{\partial s}(f_1 r_1 W) = \frac{\partial}{\partial t}\cdot[W f_1].$$

$$+ B(s)\delta(s-0) - D(s)$$

Reactor - Regenerator System



$r_1 = -k_1 s \qquad r_2 = k_2 (1-s)$

$$v_0 f_2(s)ds - v_0 f_1(s)ds + (W_1 f_1 r_1)_s - (W_1 f_1 r_1)_{s+ds} = 0$$

$$v_0 f_2 - v_0 f_1 - \frac{d}{ds}(W f_1 r_1) = 0$$

$$f_2 - f_1 - \frac{d}{ds}(f_1 r_1 \bar{t}_1) = 0 \qquad \text{Reactor. (1)}$$

$$f_1 - f_2 - \frac{d}{ds}(f_2 r_2 \bar{t}_2) = 0 \qquad \text{Regenerator (2)}$$

Add (1) and (2)

$$\frac{d}{ds}\left(f_1 r_1 \bar{t}_1 + f_2 r_2 \bar{t}_2 \right) = 0$$

$$f_1 r_1 \bar{t}_1 + f_2 r_2 \bar{t}_2 = \text{Constant} \quad — (3).$$

Integrate Eq (1)

$$1 - 1 - \left[f_1 r_1 \bar{t}_1 \right]_0^1 = 0$$

$$\left(f_1 r_1 \bar{t}_1 \right)_1 - \left(f_1 r_1 \bar{t}_1 \right)_0 = 0$$

$$\left.\begin{aligned} \left(f_1 r_1 \bar{t}_1 \right)_0 &= 0 \\ \left(f_1 r_1 \bar{t}_1 \right)_1 &= 0 \end{aligned}\right\} \quad 4 \text{ (N}$$

Integrate Eq (2)

$$1-1-\left[f_2 r_2 \bar{t}_2\right]_0^1 = 0$$

$$\left(f_2 r_2 \bar{t}_2\right)_1 - \left(f_2 r_2 \bar{t}_2\right)_0 = 0$$

$$\left.\begin{aligned}\left(f_2 r_2 \bar{t}_2\right)_1 &= 0\\ \left(f_2 r_2 \bar{t}_2\right)_0 &= 0\end{aligned}\right\} \quad 4\ (b)$$

From Eq(3)

$$f_1 r_1 \bar{t_1} + f_2 r_2 \bar{t_2} = 0$$

$$f_2 = \frac{-f_1 r_1 \bar{t_1}}{r_2 \bar{t_2}} \qquad (5).$$

Eq (1) becomes

$$-\frac{f_1 r_1 \bar{t}_1}{r_2 \bar{t}_2} - f_1 - \frac{d}{ds}\left(f_1 r_1 \bar{t}_1\right) = 0$$

$$\frac{d}{ds}\left(f_1 r_1 \bar{t}_1\right) = -f_1 r_1 \bar{t}_1 \left\{ \frac{1}{r_1 \bar{t}_1} + \frac{1}{r_2 \bar{t}_2} \right\}.$$

__Take example__

$$\alpha = 1/k_1 \bar{t}_1 = 2 \; ; \; 1/k_2 \bar{t}_2 = 3 = \beta.$$

$$\ln \frac{f_1 r_1 \bar{t}_1}{Q} = -\int \left[\frac{1}{-k_1 s \bar{t}_1} + \frac{1}{k_2 (1-s) \bar{t}_2} \right] ds$$

$$\ln \frac{f_1 r_1 \bar{t}_1}{Q} = \alpha \ln s + \beta \ln (1-s)$$

Substituting F_2

$$\ln \frac{f_1 r_1 \bar{t}_1}{Q} = \alpha \ln s + \beta \ln(1-s).$$

$$\ln \frac{f_1 r_1 \bar{t}_1}{Q} = \ln s^{\alpha} (1-s)^{\beta}$$

$$\alpha = 1/k_1 \bar{t}_1$$

$$\beta = 1/k_2 \bar{t}_2$$

$$\boxed{\frac{f_1 r_1 \bar{t}_1}{Q} = s^{\alpha} (1-s)^{\beta}}$$

$$\frac{f_1 r_1 \bar{t_1}}{Q} = s^{\alpha}(1-s)^{\beta}.$$

$$\alpha = 2, \quad \beta = 3$$

$$f_1 = -Q\alpha s^{\alpha-1}(1-s)^{\beta}$$

$$f_2 = -Q\beta s^{\alpha}(1-s)^{\beta-1}$$

$$\int_0^1 f_1\,ds = 1 = -Q\alpha \int_0^1 s(1-s)^3\,ds$$

$$1 = -Q(2)\left[\int_0^1 s(1-3s+3s^2-s^3)\,ds\right]$$

$$1 = -\varphi(2)\left[\frac{s^2}{2} - \frac{3s^3}{3} + \frac{3s^4}{4} - \frac{s^5}{5}\right]_0^1$$

$$-2\varphi\left[\frac{1}{2} - 1 + \frac{3}{4} - \frac{1}{5}\right]_0^1$$

$$-2\varphi\left[\frac{10 - 20 + 15 - 4}{20}\right]$$

$$\varphi = -10$$

$$f_1 = 10(2)s(1-s)^3$$

$$f_2 = (10)(3)s^2(1-s)^2$$

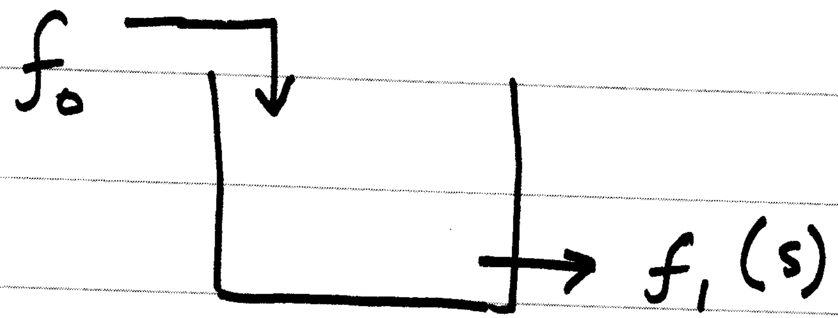
$$f_1 = 20s(1-s)^3$$

$$f_2 = 30s^2(1-s)^2$$

$$\bar{s}_1 = \int s f_1 \, ds = 20\int s^2(1-s)^3 ds = 0.33$$

$$\bar{s}_2 = \int s f_2 \, ds = 30\int s^3(1-s)^2 ds = 0.5$$

RTD of a CSTR



$$f_0 = \delta(s-0)$$

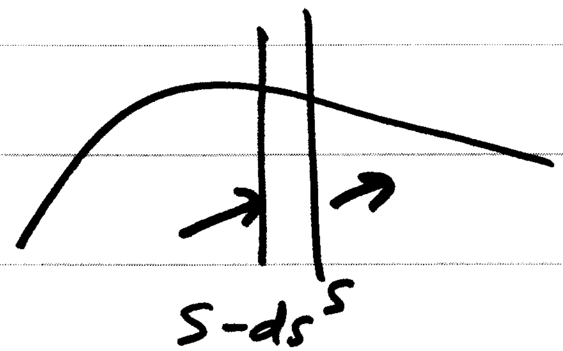
$$s = t$$

$$\cancel{f_0} - f_1 - \frac{d}{ds}\left(r_1 f_1 \bar{t}\right) = 0 \qquad \text{— (1)}$$

$$r_1 = \frac{d(\cancel{s}\ t)}{dt} = 1$$

$$- f_1 - \frac{d}{ds}\left(f_1 \bar{t_1}\right) = 0$$

$\cancel{S\to 0}$ $\quad Lt\ s \to 0$



$$f_0(s) = \delta(s-0)$$

$$1/p - 0/p + Gen = \cancel{Acc}$$

$$\underset{\substack{s\to 0\\ ds\to 0}}{Lt}\ \underbrace{\overbrace{v_0 f_0(s)\,ds}^{=1}} - \cancel{v_0 f_1(ds)} + V\left[\cancel{f_1(s-ds)}\,\cancel{r_1(s-ds)}\right] - V\left[f_1(s)\,\overset{=1}{r_1(s)}\right] = 0$$

$\cancel{v_0 f_1(s)\,ds}$

$$v_0 \cancel{s} - V\ f_1(0) \Longrightarrow \boxed{f_1(0) = 1/\bar{t}}$$

$$f_1 = Q\, e^{-s/\bar{t}}$$

$$f_1(0) = 1/\bar{t}$$

$$Q = 1/\bar{t}$$

$$\boxed{f_1 = \frac{1}{\bar{t}}\, e^{-s/\bar{t}}}$$

s: Residence time

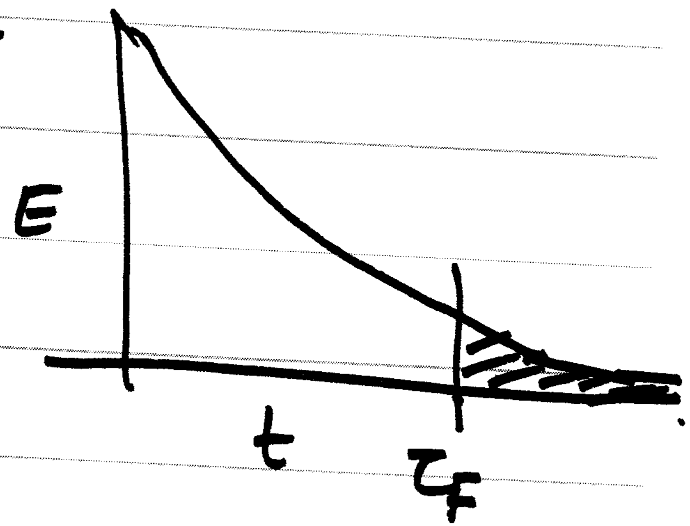
Ext Diff Contrl. gas Sld Non Cat Rxn.

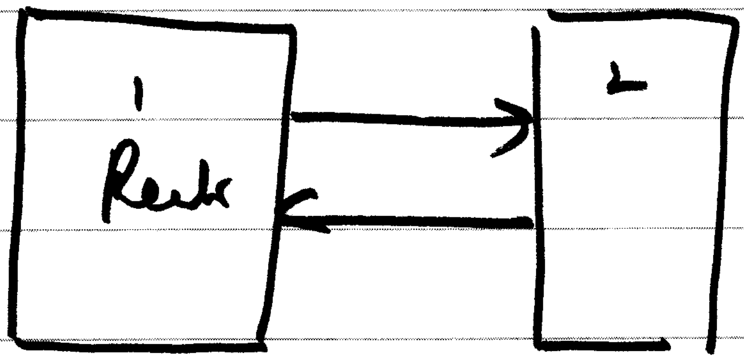
$$X_B = t/\tau_F$$

① $$\frac{d}{dt} X_B = \left(1/\tau_F\right)$$

② $$E(t) = \frac{1}{\bar{t}} e^{-t/\bar{t}}$$

$$K = \int_{\tau_F}^{\infty} E(t)\,dt = e^{-\tau_F/\bar{t}}$$





$r_1 = -k_1$ $\qquad$ $r_2 = +k_2$

Reactor.

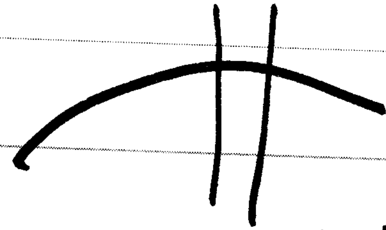
$I/p - O/p + \text{Gen} = \text{Acc}.$

$$g_2 - g_1 - \frac{d}{da} g_1 r_1 \bar{t}_1 = 0 \qquad \text{— (1). Reactr}$$

Regenerator

$$g_1 - g_2 - \frac{d}{da} g_2 r_2 \bar{t}_2 = 0 \qquad \text{— (2) Reg.}$$

<u>Reactr</u>



a a+da.

Lt $a \to 1$

$da \to 0$

I/p − O/p + Gen = 0.

$$v_0\left[\cancel{g_2\, da} + L_1\,\delta(a-1)\right]da - v_0\left[\cancel{g_1\, da} + \cancel{K_0\,\delta(a-0)}\right]da$$

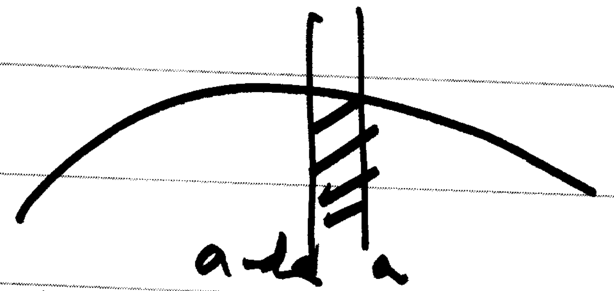
$$+\left[W r_1 g_1\right]_a - \cancel{\left[W r_1 g_1\right]_{a+da}}.$$

$$= 0.$$

$$v_0 L_1 + (W r_1 g_1)_1 = 0$$

$$(W r_1 g_1)_1 = -\,v_0 L_1 \Rightarrow (g_1 r_1 \bar{t}_1)_1 = -L_1$$

Generating the Boundary Conditions.



Reactor

$1/p - 0/p +$ Gen $=$ Acc.

Lt $a \to 0$
$da \to 0$

$$-v_0 \left[\cancel{g_1} + K_0 \delta(a-0) \right] da + v_0 \left[\cancel{g_2} + \cancel{L_1 \delta(a-1)} \right] \cancel{da}$$

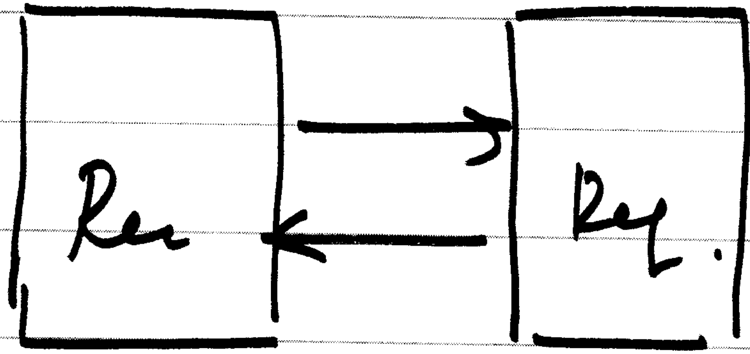
$$+ \left[W r_1 \cancel{(a-da)} \, g_1 (a-da) \right.$$

$$\left. - W (r_1(a) \, g_1(a) \right] = 0$$

$$-v_0 K_0 \delta(a-0)^{da} - (W \dot{r}_1 g_1)_0 = 0$$

$$f_2 = L_1 \delta(s-1) + g_2(s).$$

$$f_1 = K_0 \delta(s-0) + g_1(s)$$



$\cancel{r_1 = k_1}$

$r_1 = -k_1$

$r_2 = +k_2$

$$(g, r, w)_0 = -v_0 K_0$$

$$(g, r, \bar{t}_1)_0 = -K_0 \qquad (g_2\, r_2\, \bar{t}_2)_0 = +K_0$$

$$(g, r, \bar{t}_1)_1 = -L_1 \qquad (g_2\, r_2\, \bar{t}_2)_1 = +L_1$$