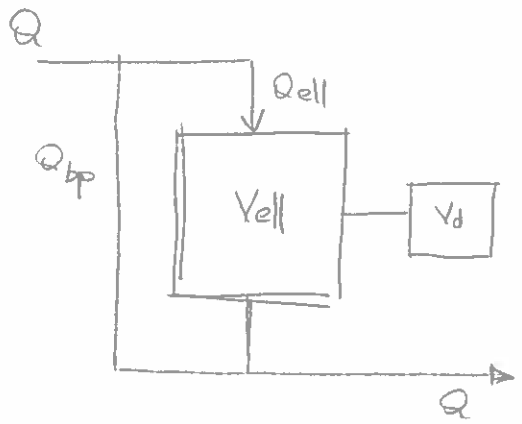
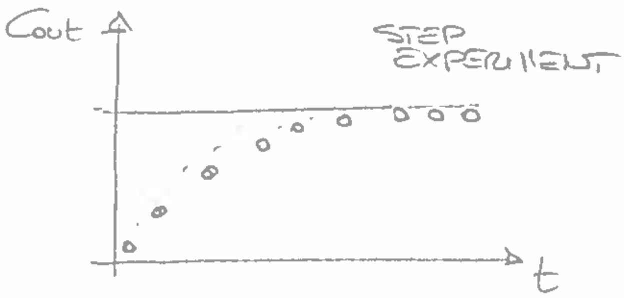
PRACTICAL SESSION 4

EXERCISE 2



compartment model
2 parameters α, β

$$\begin{cases} Q_{bp} = \alpha Q & \alpha \in [0;1] \\ V_{dead} = \beta V & \beta \in [0;1] \end{cases}$$



$$\frac{C_{OUT}}{C_0} = 1 - (1-\alpha)\, e^{-\frac{1-\alpha}{1-\beta}\frac{t}{\tau}}$$

C_0 is not given, but it can be inferred from the experimental data as the asymptotic value of the curve

linearization of tracer curve

$$\frac{C_{OUT}}{C_0} - 1 = -(1-\alpha)\, e^{-\frac{1-\alpha}{1-\beta}\frac{t}{\tau}}$$

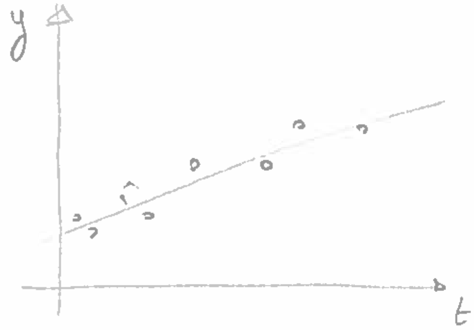
$$\frac{C_{OUT} - C_0}{C_0} = -(1-\alpha)\, e^{-\frac{1-\alpha}{1-\beta} t/\tau}$$

$$\frac{C_0}{C_{OUT} - C_0} = -\left[(1-\alpha)\, e^{-\frac{1-\alpha}{1-\beta} t/\tau}\right]^{-1}$$

$$\frac{C_0}{C_0 - C_{OUT}} = \frac{e^{\frac{1-\alpha}{1-\beta} t/\tau}}{1-\alpha}$$

$$\ln \frac{C_0}{C_0 - C_{OUT}} = \ln \frac{1}{1-\alpha} + \frac{1-\alpha}{1-\beta}\, t/\tau$$ linear model → linear regression analysis

$$\underbrace{\ln \frac{C_0}{C_0 - C_{OUT}}}_{y} = \underbrace{\ln \frac{1}{1-\alpha}}_{q} + \underbrace{\frac{1-\alpha}{1-\beta}\, t/\tau}_{m\, t}$$



$$\begin{cases} q = \ln \dfrac{1}{1-\alpha} \\ m = \dfrac{1-\alpha}{(1-\beta)\tau} \end{cases}$$

from the regression analysis

$$\underline{Y} = \left[\ln \frac{C_0}{C_0 - C_{OUT}} \right]_i = \left[\ln \frac{1}{1 - F_{exp}} \right]_i$$

$$\underline{X} = \begin{bmatrix} 1 & t_i \\ 1 & t_i \\ \vdots & \end{bmatrix} \qquad a = \begin{bmatrix} q \\ m \end{bmatrix}$$

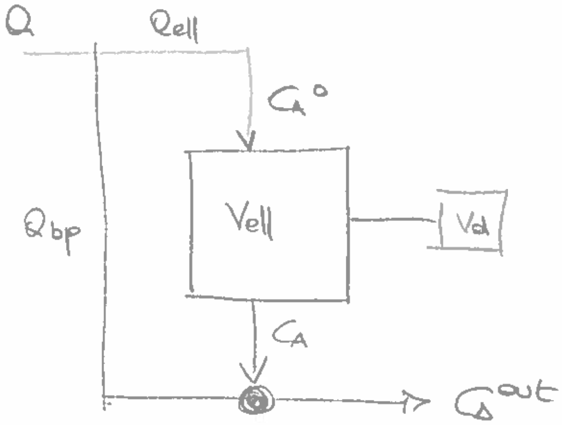
$$\underline{\underline{A}}\,\underline{a} = \underline{b} \qquad \begin{cases} \underline{\underline{A}} = \underline{\underline{X}}'\underline{\underline{X}} \\ \underline{b} = \underline{\underline{X}}'\,\underline{Y} \end{cases} \Longrightarrow$$

linear regression analysis
q, m

$$\begin{cases} \alpha = 1 - \dfrac{1}{\exp(q)} \\ \beta = 1 - \dfrac{1-\alpha}{m\tau} \end{cases}$$

complete characterization of the 2 parameter model

$$\tau_{eff} = \frac{V_{eff}}{Q_{eff}} = \frac{(1-\beta)V}{(1-\alpha)Q} = \frac{1-\beta}{1-\alpha}\,\tau$$



CSTR (τ_{ell})

$$\tau = k C_A^2$$

$$\frac{C_A^0 - C_A}{\tau_{ell}} + R_A = 0$$

$$\frac{C_A^0 - C_A}{\tau_{ell}} - k C_A^2 = 0$$

$$C_A^0 - C_A - k\,\tau_{ell}\,C_A^2 = 0$$

$$k\,\tau_{ell}\,C_A^2 + C_A - C_A^0 = 0$$

concentration at the exit of the ideal CSTR

$$C_A = \frac{-1 + \sqrt{1 + 4k\,\tau_{ell}\,C_A^0}}{2k\,\tau_{ell}}$$

outlet concentration

$$Q\,C_A^{out} = Q_{ell}\,C_A + Q_{bp}\,C_A^0$$

$$C_A^{out} = (1-\alpha)\,C_A + \alpha\,C_A^0$$

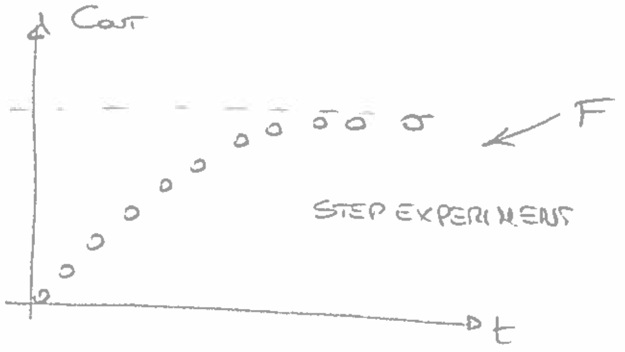
$$\boxed{C_A^{out} = (1-\alpha)\,\frac{-1 + \sqrt{1 + 4k\,\tau_{ell}\,C_A^0}}{2k\,\tau_{ell}} + \alpha\,C_A^0}$$

Comparison with the ideal CSTR behavior

$$C_A^{CSTR} = \frac{-1 + \sqrt{1 + 4k\,\tau\,C_A^0}}{2k\,\tau}$$

the only difference with respect to C_A from the effective CSTR above is the residence time τ vs τ_{ell}

EXERCISE 3



Segregation model

from the CDF F we have to infer the RTD E

we can proceed in two different ways:

1) numerical differentiation of F to have E (inaccuracies can arise)
2) fitting of F with a proper non linear function and then analytical differentiation

If we look qualitatively at the shape of F we can imagine that the reactor has a mixed flow like behavior, so we can try to see if we can use the following fitting function with 2 parameters C_2 and C_3

$$F(t) = 1 - C_2 \exp\left(-\frac{t}{C_3}\right)$$

in case of perfect CSTR $C_2 = 1$, $C_3 = \tau$

even if a linear regression is possible, we can also proceed using non linear regression tools

<u>linear regression</u>

$$1 - F = C_2 \exp\left(-\frac{t}{C_3}\right)$$

$$\underbrace{\ln(1-F)}_{y} = \underbrace{\ln C_2}_{q} \underbrace{- \frac{1}{C_3} t}_{m t}$$

$$\begin{cases} y = 1 - F \\ m = -\frac{1}{C_3} \\ q = \ln C_2 \end{cases}$$

Residence time Distribution function

$$E = \frac{dF}{dt}$$

$$\boxed{E = \frac{C_2}{C_3} \exp\left(-\frac{t}{C_3}\right)}$$

Segregated model

$$C_A^{out} = \int_0^{\infty} C_A^{batch}(t)\, E(t)\, dt$$

we need to find the expression of evolution in a batch reactor

$$\begin{cases} \dfrac{dC_A^{batch}}{dt} = -k\, C_A^{batch\,2} \\ C_A^{batch}(t=0) = C_A^0 \end{cases}$$

$$C_A^{batch\,-2}\, dC_A^{batch} = -k\,dt$$

$$C_A^{batch}(t) = \frac{C_{A0}}{1 + k t C_{A0}}$$

$$C_A^{out} = \underbrace{\int_0^{\infty} \frac{C_{A0}}{1 + k t C_A^0} \cdot \frac{C_2}{C_3} \exp\left(-\frac{t}{C_3}\right) dt}_{\text{numerical integration}}$$

Comparison with PFR and CSTR

$$C_{CSTR}^{out} = \frac{-1 + \sqrt{1 + 4k\tau C_A^0}}{2k\tau}$$

$$C_{PFR}^{out} = \frac{C_{A0}}{1 + k\tau C_{A0}}$$

EXERCISE 4

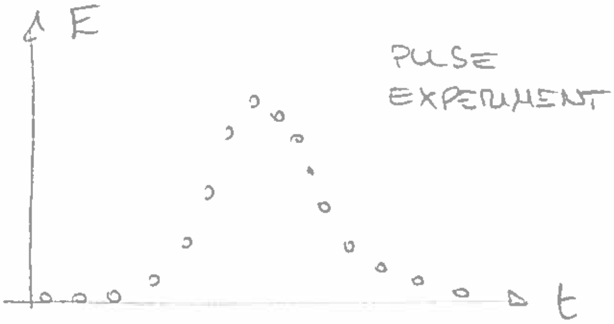
We can find the RTD exactly following the same steps in the previous exercise

Maximum Mixedness Model

$$\begin{cases} \dfrac{dC_A}{d\lambda} = \dfrac{E}{1-F}\left(C_A - C_A^0\right) - R_A \\ C_A(\lambda \to \infty) = C_A^0 \end{cases}$$

$\lambda \to \infty$ can be replaced with the maximum value of λ we can expect in our system

EXERCISE 1



It is important to be sure that the area below the curve E is equal to 1 i.e. that the E curve is normalized

$$M_0 = \int_0^\infty E(t)\,dt = 1$$

mean residence time

$$t_m \stackrel{\text{def}}{=} \int_0^\infty t\,E(t)\,dt$$

(this is also m_1)

calculation of variance

$$m_2 = \int_0^\infty t^2 E(t)\,dt$$

$$\sigma^2 = m_2 - t_m^2 \qquad \sigma_\theta^2 = \frac{\sigma^2}{t_m^2}$$

DISPERSION MODEL

$$\sigma_\theta^2 = \frac{2}{Pe}\left[1 - \frac{1}{Pe}\left(1 - e^{-Pe}\right)\right]$$

if $Pe \gg 1$

$$\sigma_\theta^2 = \frac{2}{Pe} \Rightarrow Pe = \frac{2}{\sigma_\theta^2}$$

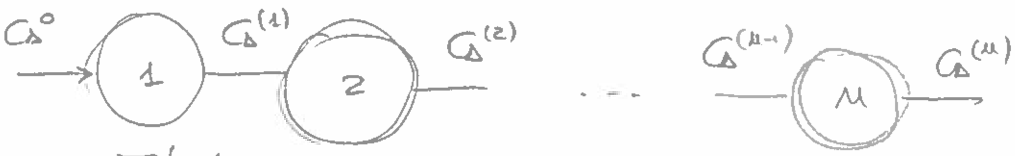
iterative procedure

$$Pe^{(k+1)} = \frac{2}{\sigma_\theta^2}\left[1 - \frac{1}{Pe^{(k)}}\left(1 - e^{-Pe^{(k)}}\right)\right]$$

Effective dispersion coefficient $\quad D_{eff} = \frac{Lv}{Pe}$

TANKS IN SERIES MODEL

$$n = \frac{1}{\sigma_\theta^2}$$



$$\tau' = \frac{t_m}{n}$$

$$C_A^{(k)} = \frac{-1 + \sqrt{1 + 4k\tau' C_A^{(k-1)}}}{2k\tau'} \qquad k = 1 \ldots n$$

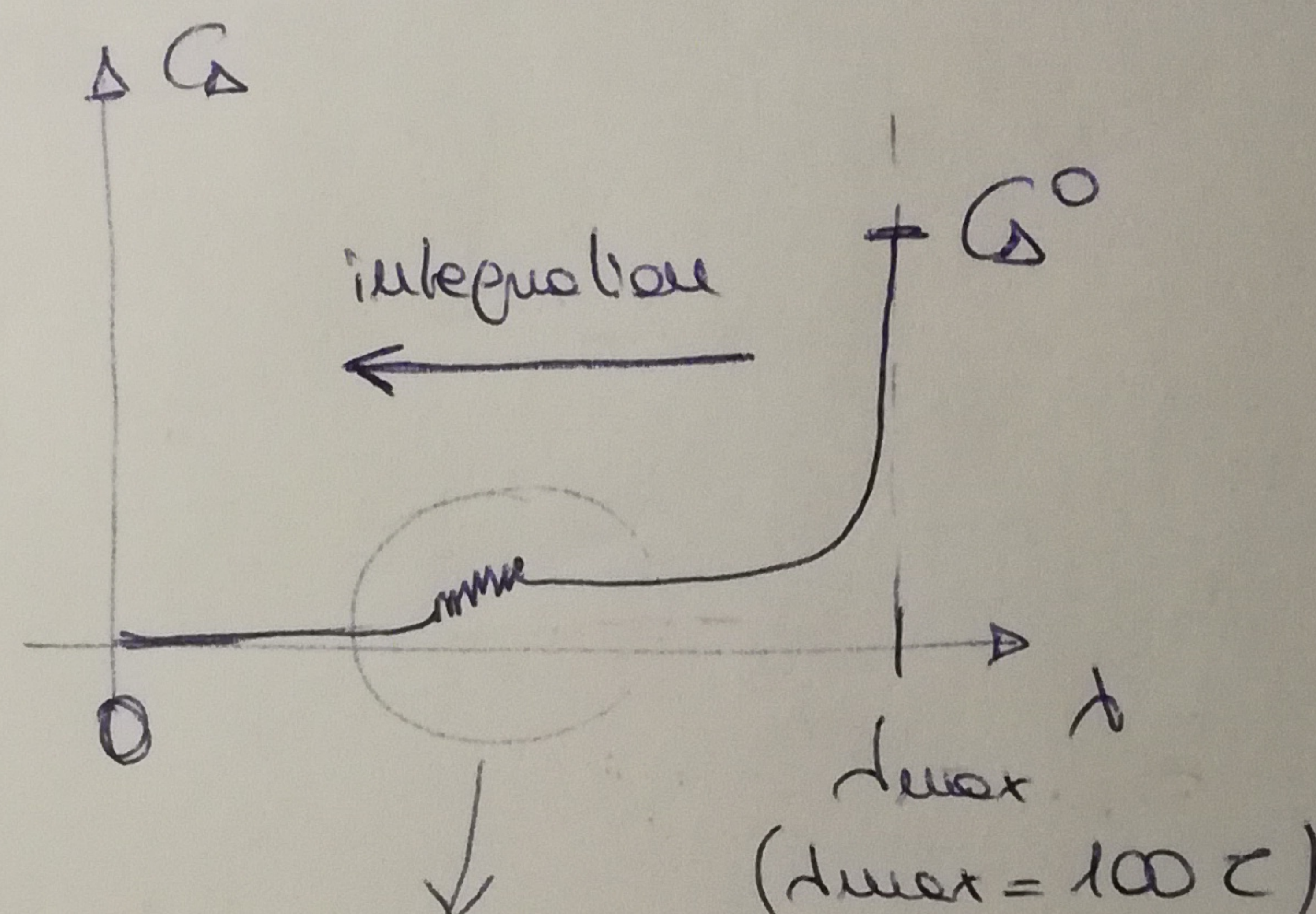
PRACTICAL SESSION 5
EXERCISE 4

$$\begin{cases} \dfrac{dC_A}{dt} = \dfrac{E}{1-F}\left(C_A - C_A^{in}\right) - R_A \\ C_A(t = t_{max}) = C_A^0 \end{cases}$$

Problem: $\begin{cases} \lim_{t\to 0} E = 0 \\ \lim_{t\to 0} (1-F) = 0 \end{cases} \rightarrow$ if $t \to 0$ $\dfrac{E}{1-F} \simeq \dfrac{0}{0}$??

numerical problems

Example:



here $\dfrac{E}{1-F} \simeq \dfrac{0}{0}$ from this point the solution is wrong

Solution: just use the analytical expression of $\dfrac{E}{1-F}$

$$E = \frac{C_2}{C_3}\exp(-t/C_3)$$

$$1-F = 1-\left(1-C_2\exp\left(-\frac{t}{C_3}\right)\right) = C_2\exp(-t/C_3)$$

$$\frac{E}{1-F} = \frac{C_2}{C_3}\,\frac{\exp(-t/C_3)}{C_2\exp(-t/C_3)} = \frac{1}{C_3} \;!$$

no numerical issues, $\dfrac{E}{1-F}$ is always numerically ok!