EXERCISE 2

compartment model
2 parameters α, β

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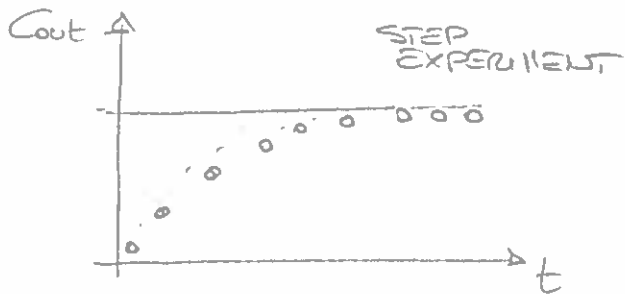
STEP EXPERIMENT

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

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

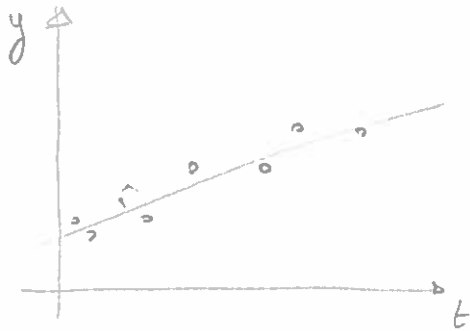$$\frac{C_{OUT}}{C_0} - 1 = -(1-\alpha) e^{-\frac{1-\alpha}{1-\beta} \frac{t}{\tau}}$$

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

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

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

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

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

$$\begin{cases} q = \ln \frac{1}{1-\alpha} \\ \\ m = \frac{1-\alpha}{(1-\beta)\tau} \end{cases} \quad \text{from the regression analysis}$$
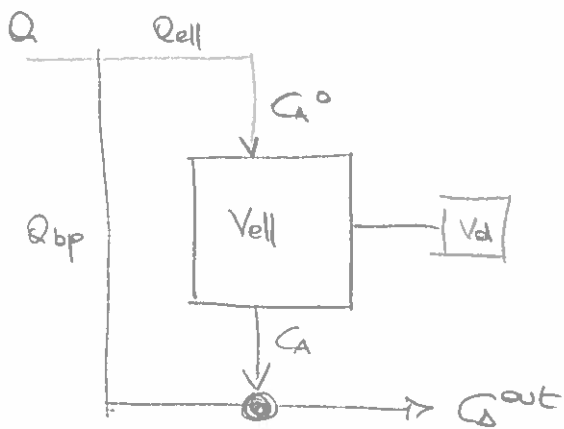
$$\underline{Y} = \left[\ln \frac{C_0}{C_0 - C_{out}} \right]_i = \left[\ln \frac{1}{1-F_{exp}} \right]_i$$

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

$$\underline{\underline{A}} \, \underline{a} = \underline{b} \qquad \begin{cases} \underline{\underline{A}} = \underline{\underline{X}}' \underline{\underline{X}} \\ \underline{b} = \underline{\underline{X}}' \underline{Y} \end{cases} \quad \Longrightarrow \quad \begin{array}{c} \text{linear regression} \\ \text{analysis} \\ q, m \end{array}$$

$$\begin{cases} \alpha = 1 - \frac{1}{\exp(q)} \\ \\ \beta = 1 - \frac{1-\alpha}{m\tau} \end{cases} \quad \begin{array}{c} \text{complete characterisation} \\ \text{of the 2 parameter model} \end{array}$$

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

$$CSTR \; (\tau_{ell})$$

$$\tau = K C_A^2$$

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

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

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

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

concentration
at the exit of
the ideal CSTR

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

outlet concentration

$$Q C_A^{out} = Q_{ell} C_A + Q_{bp} C_A^0$$
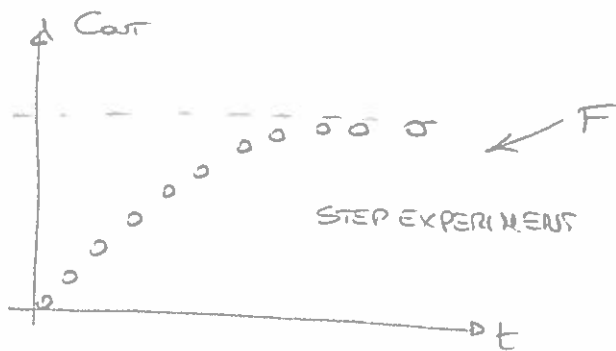
$$C_A^{out} = (1 - \alpha) C_A + \alpha C_A^0$$

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

Comparison with ideal CSTR behaviour

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

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

EXERCISE 3

STEP EXPERIMENT

Sequepolicau 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)

$\Longrightarrow$ 2) filling 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 behaviour, 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

linear regression

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

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

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

Residence time Distribution function

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

Segregated model

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

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

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

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

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

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

numerical integration

Comparison with PFR and CSTR

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

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

EXERCISE 4

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

Maximum Mixedness Model $\left\{ \begin{array}{l} \dfrac{dC_A}{d\lambda} = \dfrac{E}{1-F}(C_A - C_A^0) - R_A \\[2mm] C_A(\lambda \to \infty) = C_A^0 \end{array} \right.$

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

EXERCISE 1

PULSE EXPERIMENT

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
$$t_m \overset{def}{=} \int_0^\infty t\,E(t)\,dt \qquad (\text{this is also } m_1)$$

calculation of variance
$$M_2 = \int_0^\infty t^2\,E(t)\,dt$$

$$\sigma^2 = M_2 - t_m^2 \qquad\qquad \sigma_\theta^2 = \dfrac{\sigma^2}{t_m^2}$$

DISPERSION MODEL

$$\sigma_\theta^2 = \dfrac{2}{Pe}\left[1 - \dfrac{1}{Pe}(1 - e^{-Pe})\right] \qquad\qquad \text{if } Pe \gg 1$$

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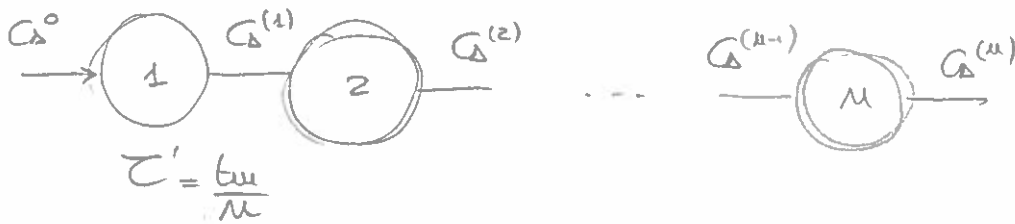
iterative procedure
$$Pe^{(k+1)} = \dfrac{2}{\sigma_\theta^2}\left[1 - \dfrac{1}{Pe^{(k)}}(1 - e^{-Pe^{(k)}})\right]$$

Effective dispersion
coefficient

$$\Gamma_{ell} = \frac{L \, v}{Pe}$$

TANKS IN SERIES MODEL

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

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

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

$$\left\{ \begin{array}{l} \dfrac{dc_A}{d\lambda} = \dfrac{E}{1-F}\left(c_A - c_A^{in}\right) - R_A \\[4mm] c_A(\lambda = \lambda_{max}) = c_A^0 \end{array}\right.$$

Problem :

$$\left\{ \begin{array}{l} \lim\limits_{\lambda \to 0} E = 0 \\[3mm] \lim\limits_{\lambda \to 0} (1-F) = 0 \end{array}\right. \longrightarrow \text{ if } \lambda \to 0 \quad \dfrac{E}{1-F} \approx \dfrac{0}{0} \quad ??$$
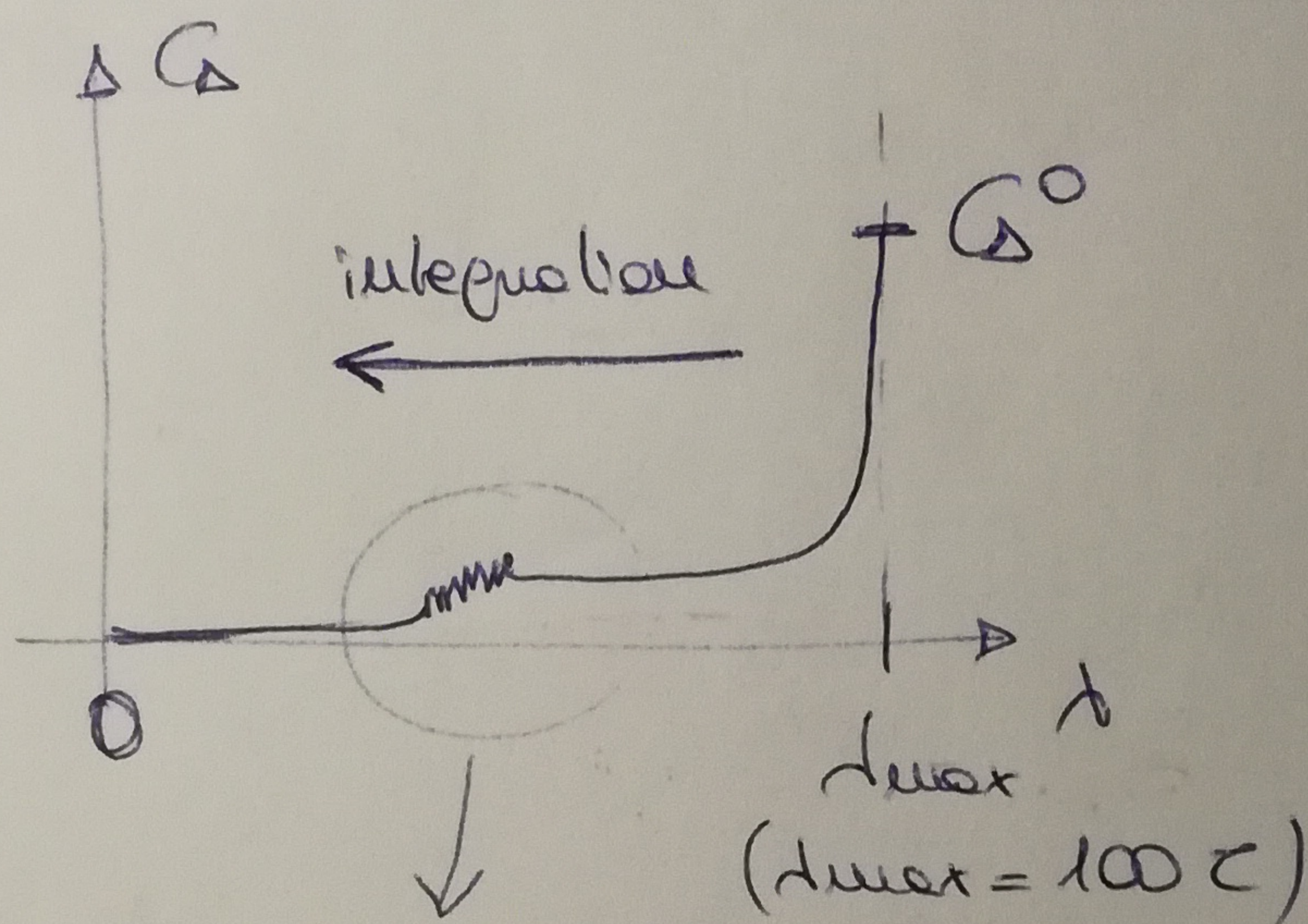
↘ numerical problems

Example :

$(\lambda_{max} = 100\,c)$

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

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

$$E = \dfrac{C_2}{C_3} \exp\left(- t/C_3\right)$$

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

$$\dfrac{E}{1-F} = \dfrac{C_2}{C_3} \dfrac{\exp(-t/C_3)}{C_2 \exp(-t/C_3)} = \dfrac{1}{C_3} \quad !$$

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