

Given RTD Data (t, C)

- 1) Model using r.p. or c.s.
- 2) Normalize to get $E(t)$
- 3) Zero out terminal ranges $\Rightarrow E(t)$

Given input data (t, C)

- 1) Model using r.p. or c.s.
- 2) Zero out terminal ranges $\Rightarrow C_{in}(t)$

Integrate convolution of $C_{in}(t) + E(t)$

$$\begin{aligned} C_{out}(t) &= \int_0^t C_{in}(t-t') E(t') dt' \\ &= \int_0^t C_{in}(t') E(t-t') dt' \end{aligned}$$



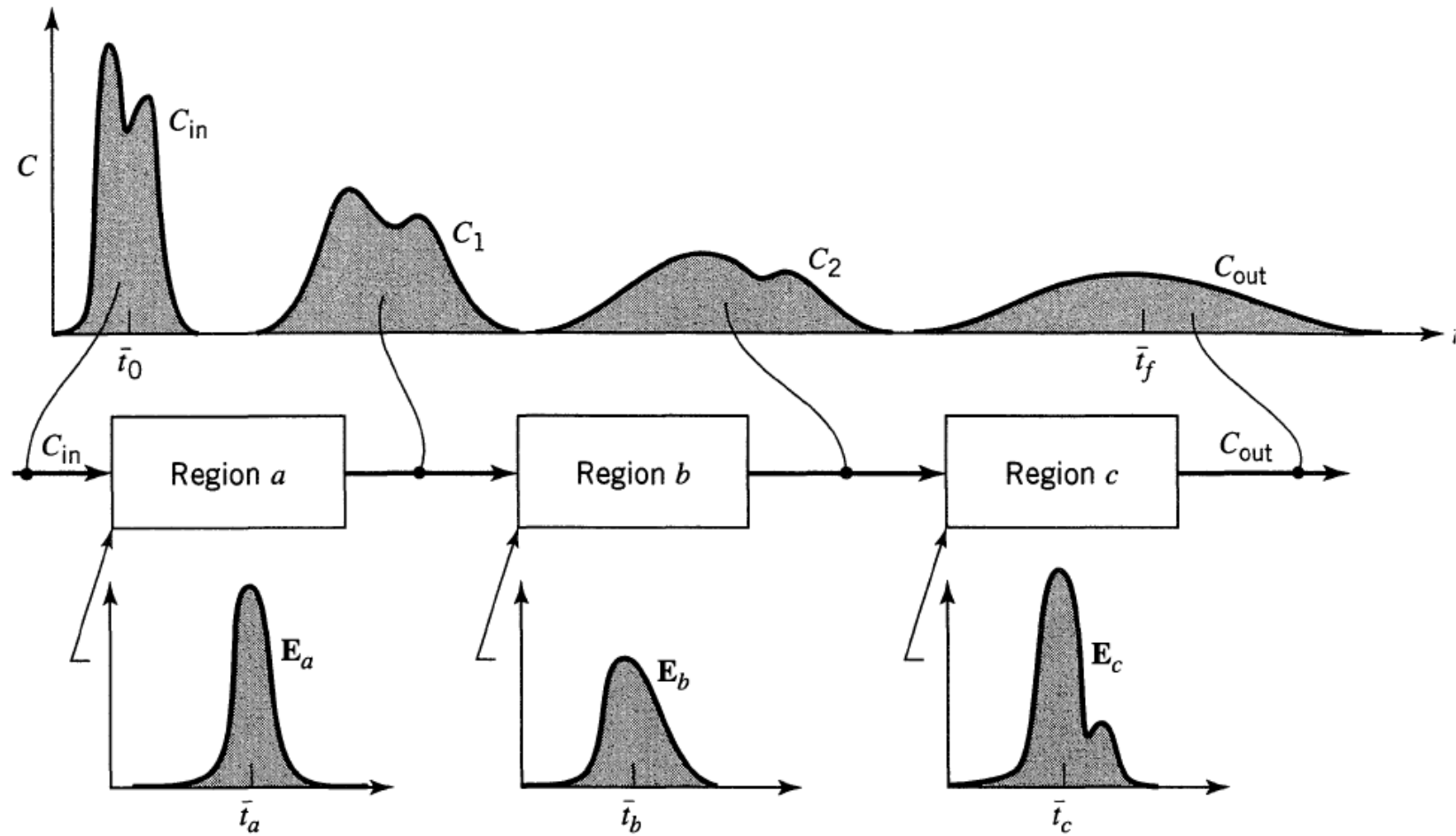


Figure 11.16 Modification of an input tracer signal C_{in} on passing through three successive regions.

- If the input signal C_{in} is measured and the exit age distribution functions E_a , E_b , and E_c are known, then C_1 is the convolution of E_a with C_{in} and so on, thus

$$C_1 = C_{in} * \mathbf{E}_a, \quad C_2 = C_1 * \mathbf{E}_b, \quad C_{out} = C_2 * \mathbf{E}_c$$

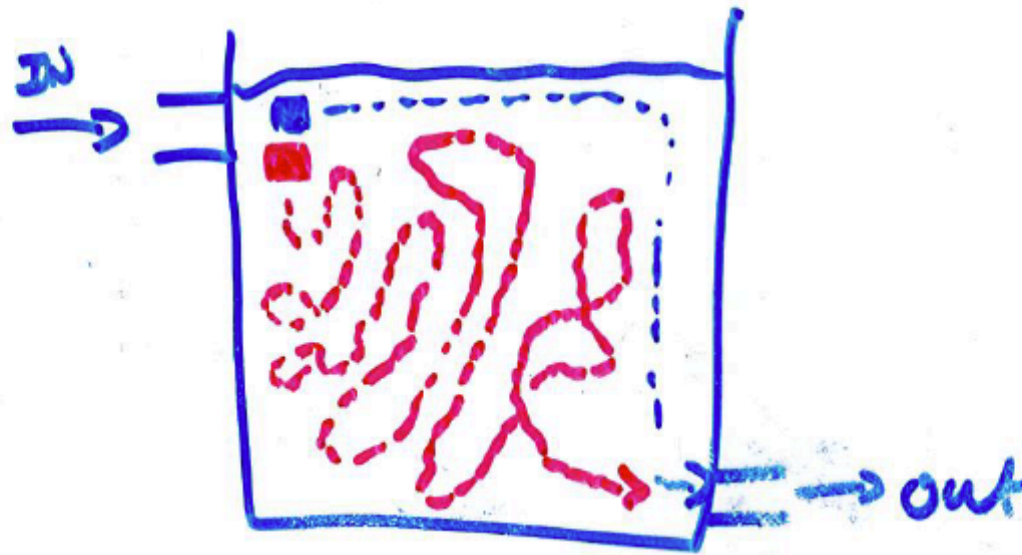
and on combining

$$C_{out} = C_{in} * \mathbf{E}_a * \mathbf{E}_b * \mathbf{E}_c \quad (11)$$

Thus we can determine the output from a multiregion flow unit.

RTD

Concept: Elements of fluid entering a reactor follow different paths to exit, \therefore there is a distribution of residence times for outlet flow elements



Non-ideal flow

⇒ How does non-ideal flow affect conversion in reactors?



$$r = f(c)$$

$$X = g(c)$$

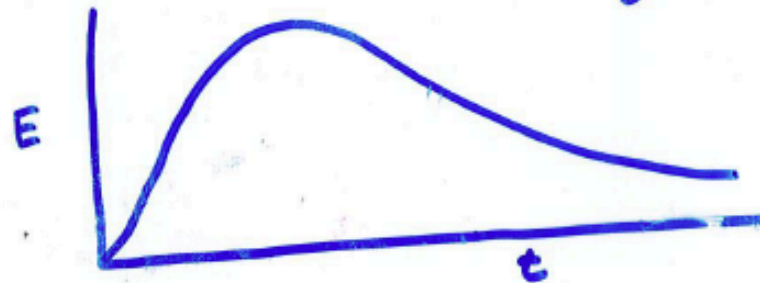
$$\tau = h(c)$$



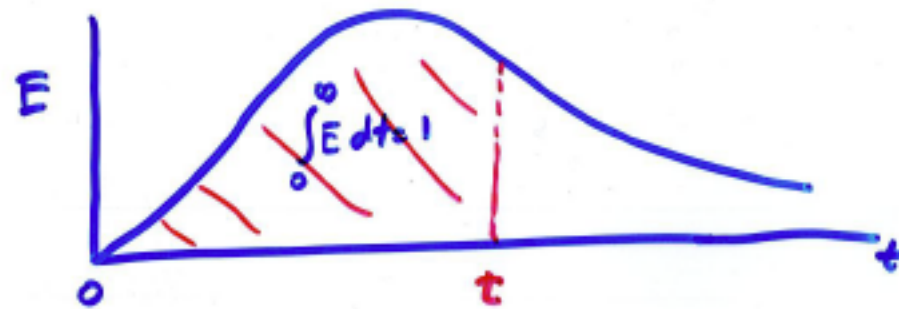
ONLY FLOW



Residence time distribution $\int_0^{\infty} E dt = 1$



E = exit age distribution



$\int_0^t E dt =$ % of exiting fluid that has spent less than t in reactor

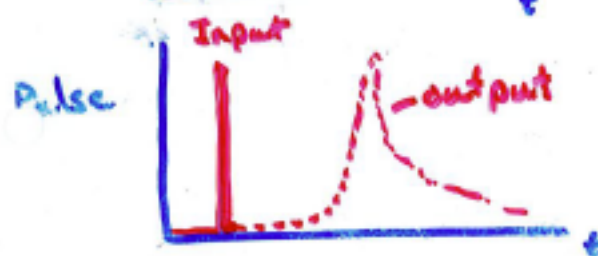
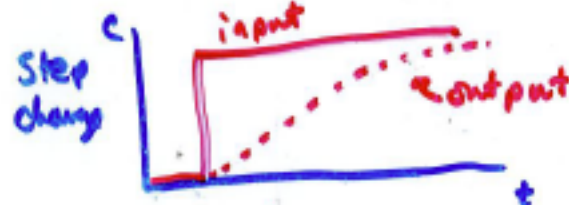
Note: $E(t) \geq \frac{1}{t}$

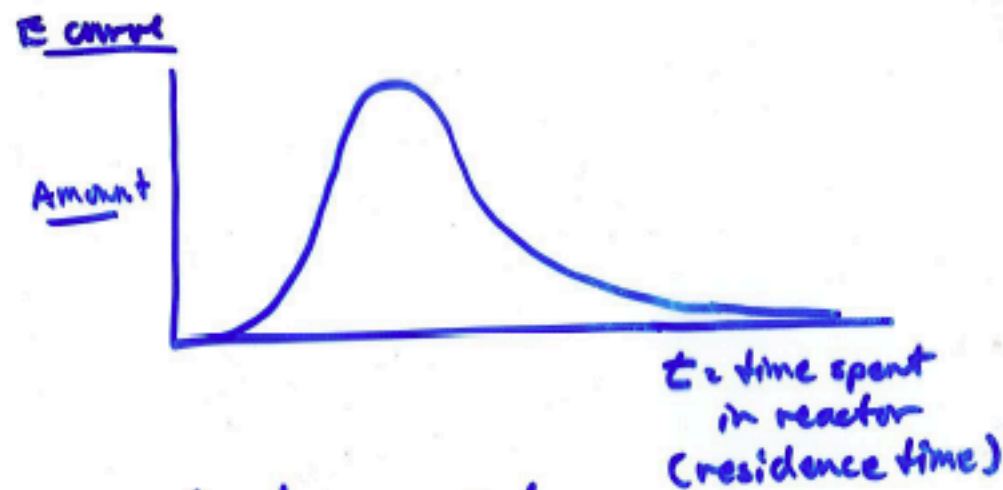
How to get $E(t)$

tracer



measure tracer output vs. time





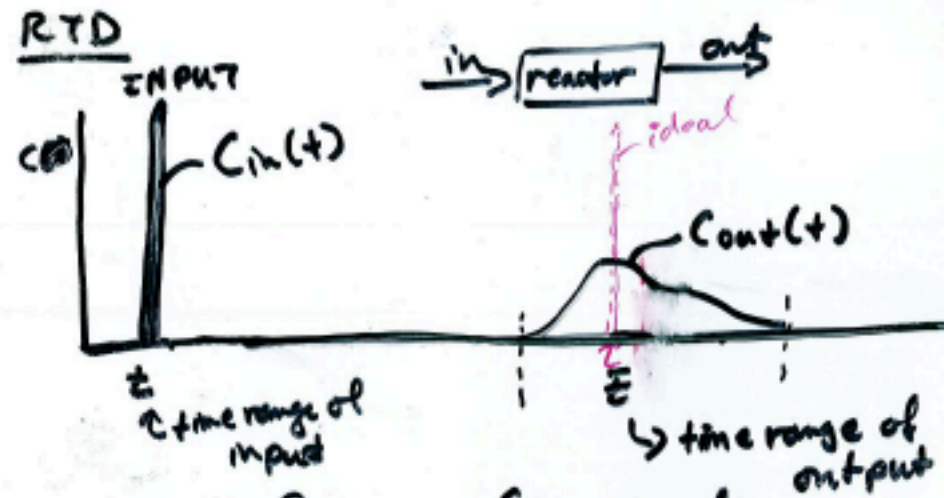
If normalized so area under curve = 1, this is called the exit age distribution or E curve.

$$\int_0^{\infty} E(t) dt = 1$$

$$\int_{t'}^{\infty} E dt = ? \text{ fluid that exits after } t'$$



$$\int_0^{t'} E dt = ? \text{ of fluid that takes less than } t' \text{ to exit reactor}$$



mass balance: $\int C_{in}(t) dt = \int C_{out}(t) dt$

$$\bar{t} = \frac{\int t C_{out}(t) dt}{\int C_{out}(t) dt} \quad (= \tau \text{ for ideal reactor})$$

$$E(t) = \frac{C_{out}(t)}{\int C_{out}(t)}$$

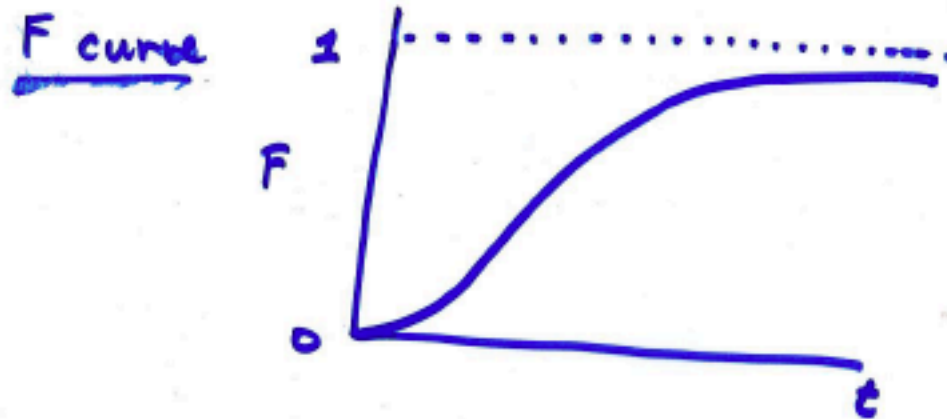
\Rightarrow output curve normalized
to total area = 1

$\int_{t_i}^{t_e} C_{out}(t) dt$

$\int_0^\infty C_{out}(t) dt$

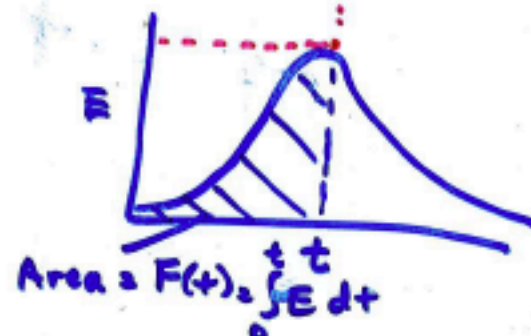
$= \frac{\text{area under curve}}{\text{total area}} = \frac{\text{fraction of material exiting}}{\text{total material exiting}}$

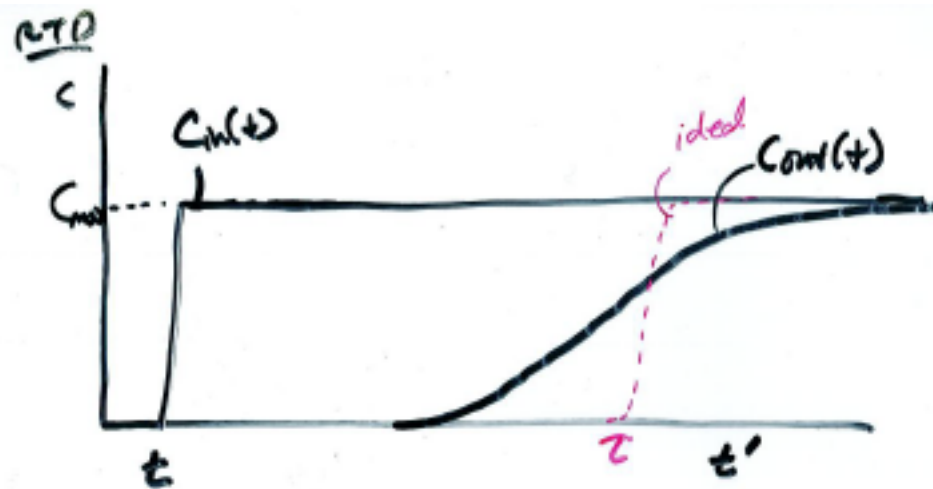
Example 11.1



F(t) % of material entering that has exited by time t

$$F = \int_0^t E \, dt \quad \text{or} \quad \frac{dF}{dt} = E$$

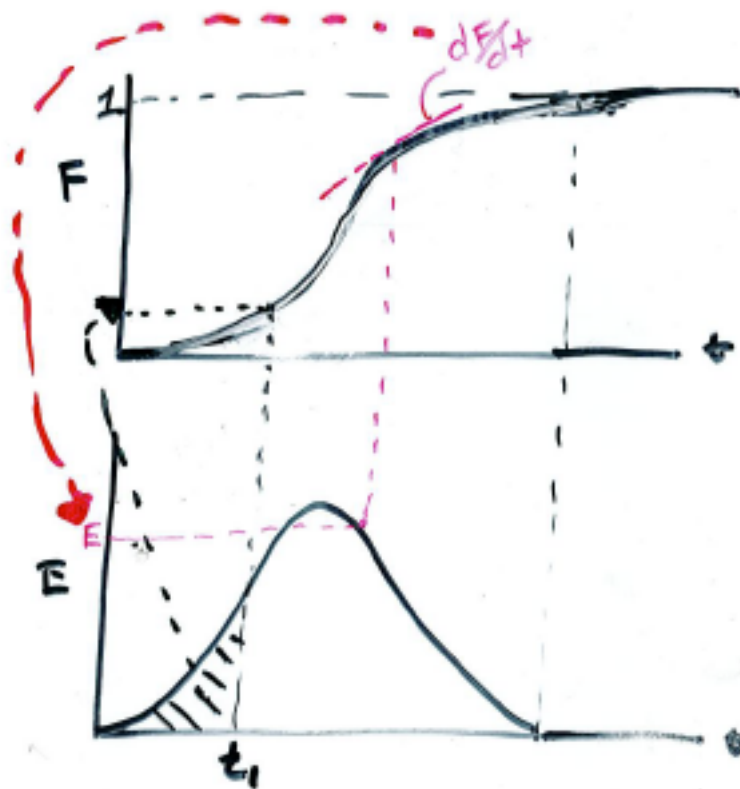




Normalise: $F = \frac{c}{c_{max}} \Rightarrow 0 \leq F \leq 1$



$F(t) = \frac{\% \text{ of new fluid}}{100}$



$$F = \int_0^{t_1} E dt$$

or

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

$$F = \text{? of material exiting}$$

$$= \int E dt$$

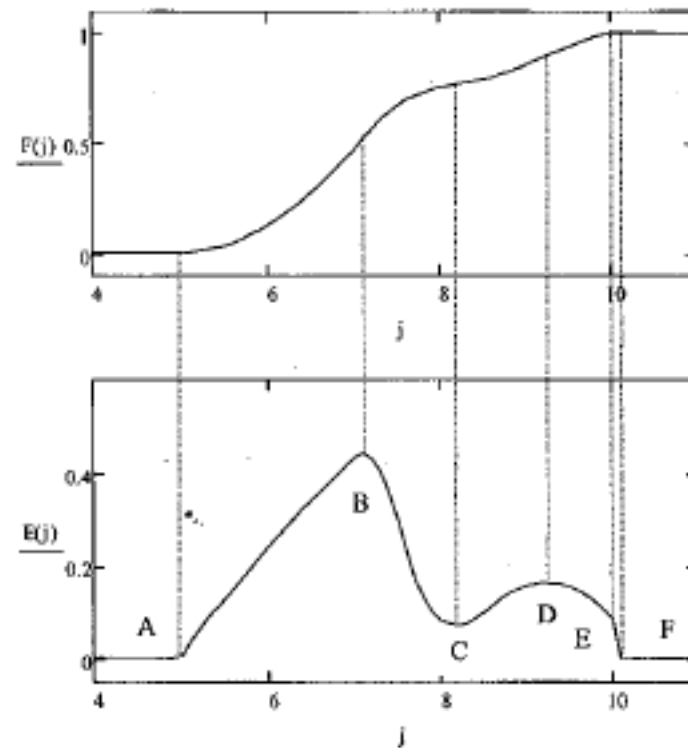
Step input

$$\bar{t} = \frac{\int_0^{C_{max}} t dC}{\int_0^{C_{max}} dC} = \frac{\int_0^1 t dF}{\int_0^1 dF} = \int_0^1 t dF$$

CAN Model $E(t) + F(t)$ from
 $C(t)$ data.

- ⇒ Regression polynomials ⇒ $R(t)$
- ⇒ Cubic splines ⇒ $S_i(t)$

Can differentiate + integrate
both $R(t)$ & $S_i(t)$ models.



A – start of output response, note relative shapes of E and F curves with time

B – maximum point of E ($dE/dt = 0$), inflection point of F ($dF/dt = d^2F/dt^2 = 0$)

C – minimum point of E ($dE/dt = 0$), inflection point of F ($dF/dt = d^2F/dt^2 = 0$)

D – maximum point of E ($dE/dt = 0$), inflection point of F ($dF/dt = d^2F/dt^2 = 0$)

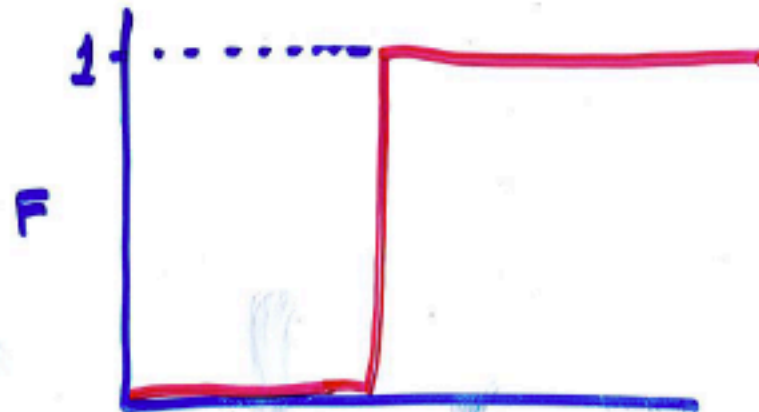
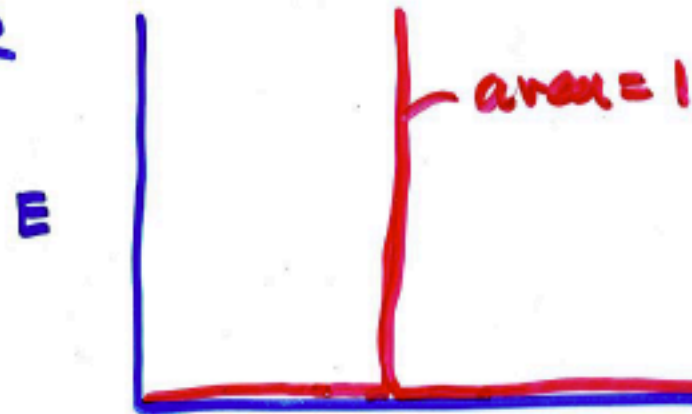
E – sharp drop in E curve, flattens out F curve

F – output response stops, E goes to zero, F goes to 1 (remains there for increasing t)

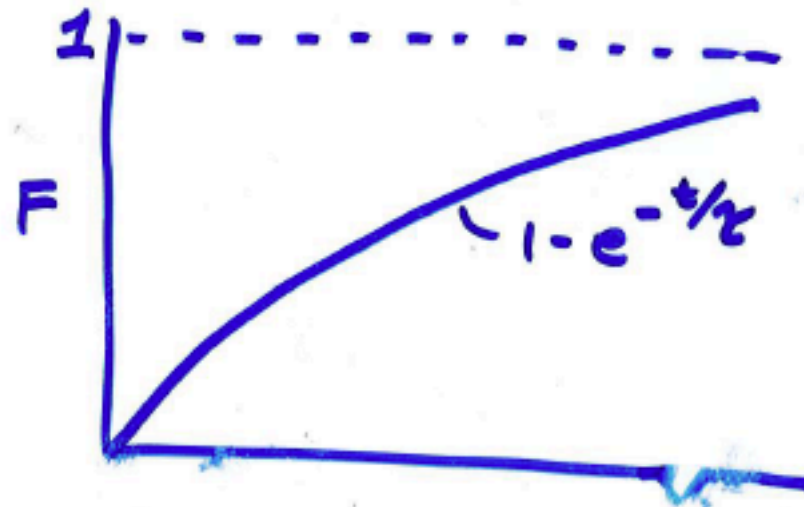
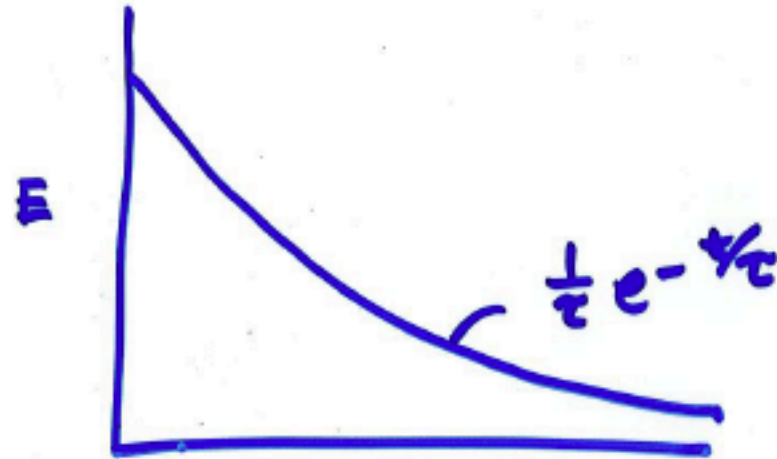
Ideal flow systems



PFR



MFR

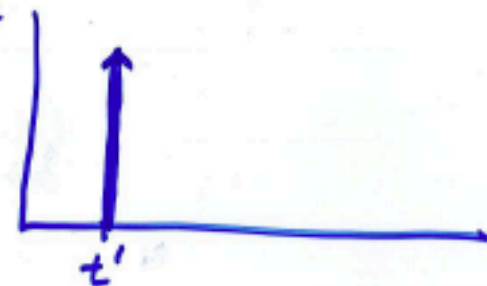


Ideal
PFR

Pulse input

$t \neq t' \quad C = 0$

$t = t' \quad \text{pulse}$
 $\int C dt = 1$



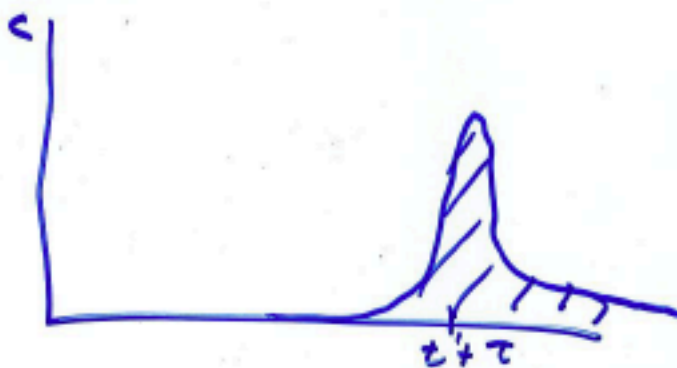
$t \neq t' + \tau \quad C = 0$

$t = t' + \tau$
 $\int C dt = 1$



What would non-ideal flow
look like?

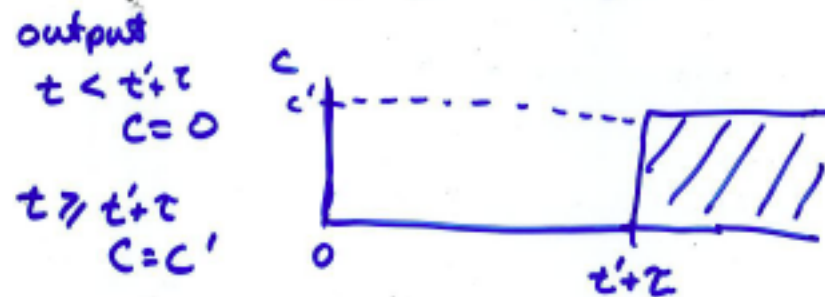
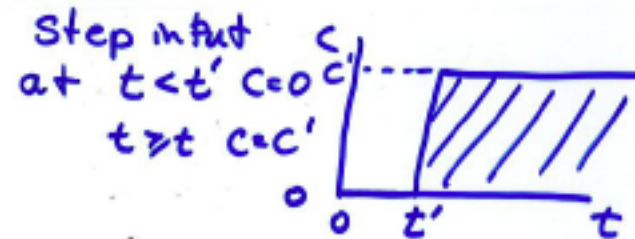
$\int C dt = ?$



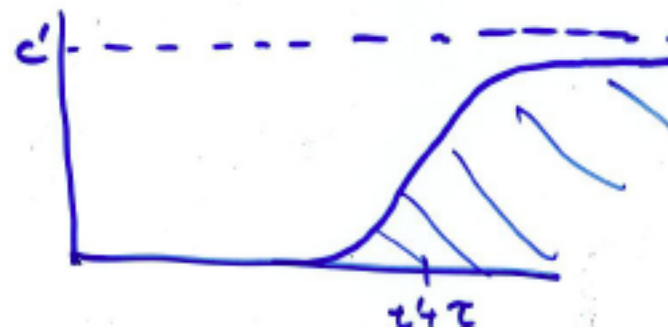
Methods to test/visualize nonideality (mixing) only
 ideal PFR



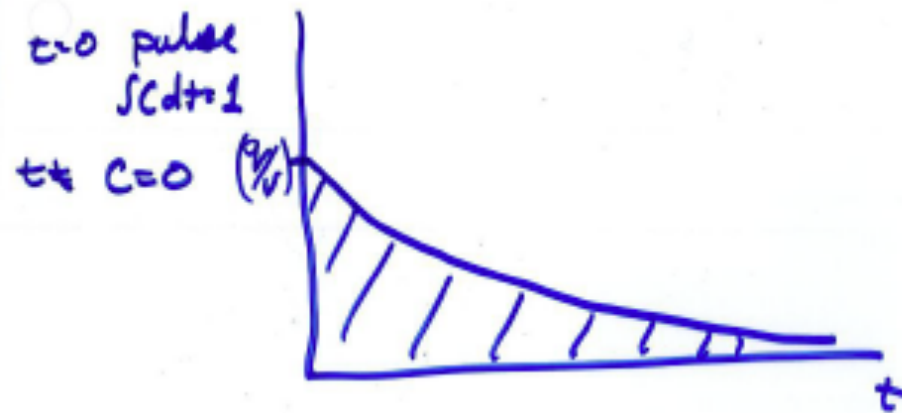
Ideal



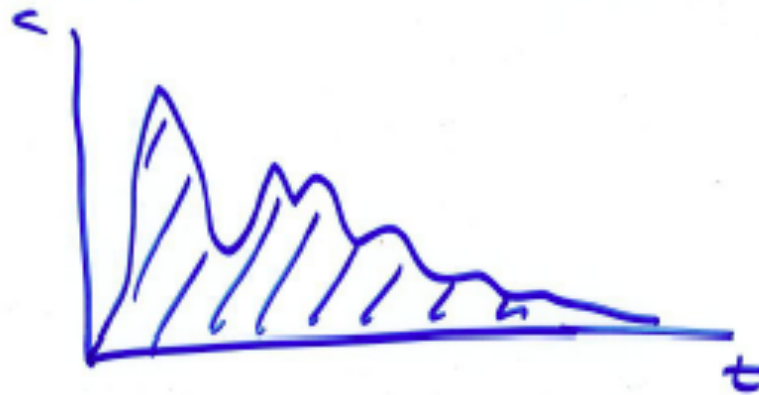
What would Non-ideal flow look like?



Pulse input, MFR



What would non-ideal look like?

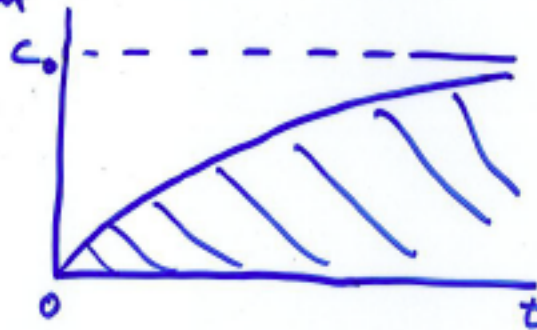


MFR

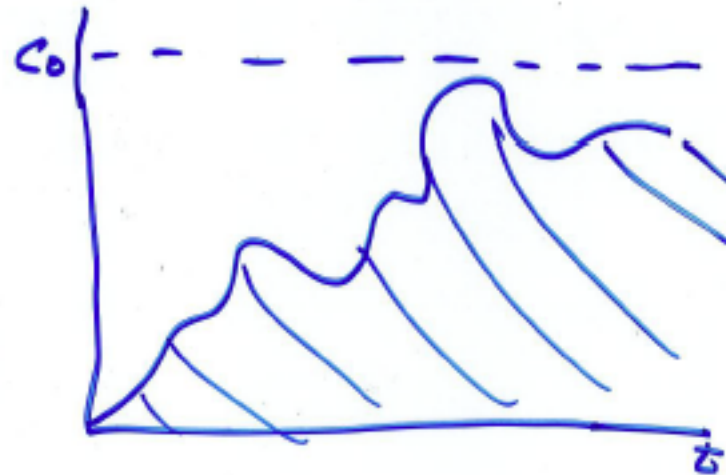
step input

$$t=0 \quad C=0$$
$$C_{in} = C_0$$

$$t>0 \quad C=C_{out}$$



what would non-ideal mixing look like?



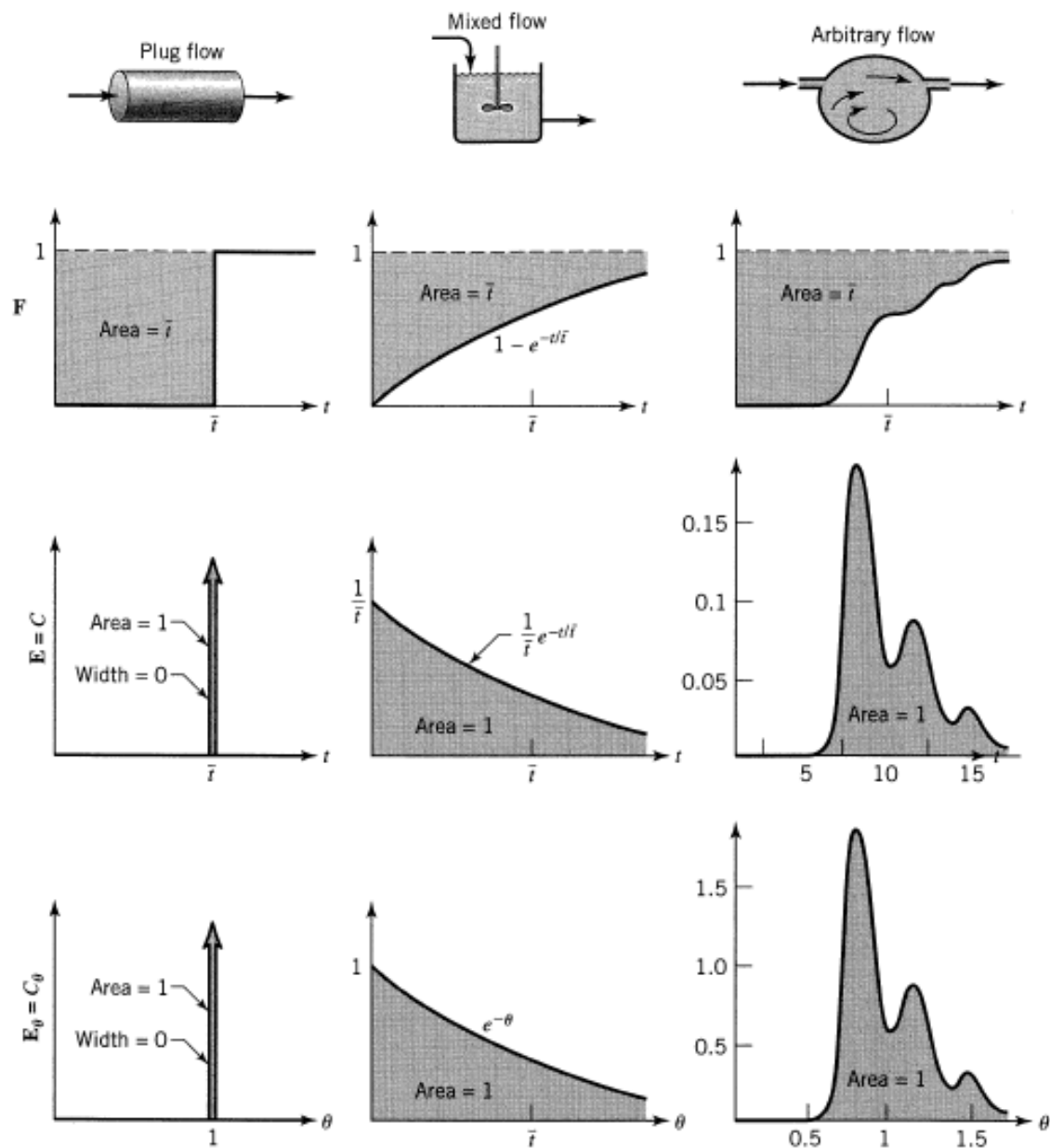


Figure 11.14 Properties of the E and F curves for various flows. Curves are drawn in terms of ordinary and dimensionless time units. Relationship between curves is given by Eqs. 7 and 8.

Developing models for ideal reactor mixing

PFR \Rightarrow initial, ~~any~~ input signal only
time displaced

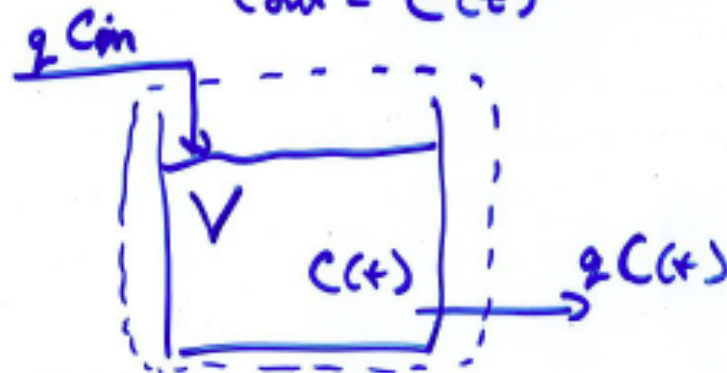
MFR

step input $t=0$ $C=0$ $C_{in} = C_0$

Ideal MFR

Reactor contents homogenous,
perfectly mixed

$$C_{out} = C(t)$$



Derive $C(t) = f(t, \tau)$



Step function $t=0$ $C=0$ (start C_0)
 $t=t$ $C=C$

$$qC_0 - qC = V \frac{dC}{dt} \quad (\text{No rxn! just mixing})$$

$$\int_0^t dt = \int_0^C \frac{V}{q(C_0 - C)} dC$$

$$t = -\tau \ln(C_0 - C) \Big|_0^C$$

$$= -\tau \ln\left(\frac{C_0 - C}{C_0}\right)$$

$$e^{-t/\tau} = \frac{C_0 - C}{C_0} = 1 - C/C_0$$

$$C/C_0 = 1 - e^{-t/\tau}$$