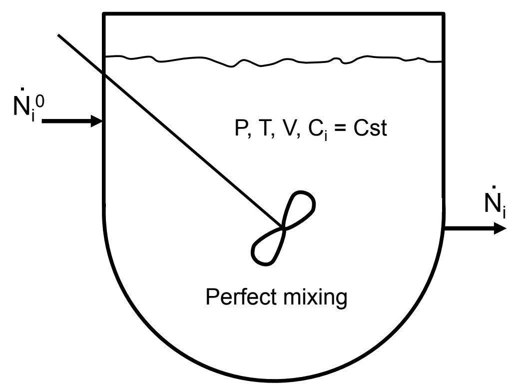
ChE-403 Problem Set 1.3

Week 3

Problem 1

A) Can you derive/calculate E(t) for a CSTR?

B) Can you use E(t) to calculate $\bar{t}$?



Hint: you measure E(t) by injecting a tracer and measuring the output concentration. Can you calculate what C(t) is for a CSTR if you inject a known number of moles of a tracer (N_t^0) at t = 0

You will also need the following integral identity: $\int_0^\infty x \exp(-x)\, dx = 1$

Solution:

a) @ $t = 0$ the tracer is perfectly mixed/diluted: $C(t = 0) = \frac{N^0}{V_R} = C^0$

After injection the mass balance on the tracer is:

Acc. = In – Out +Source

$$\frac{dN}{dt} = 0 - \dot{N} + 0$$

$$V = cst \quad \dot{V} = cst$$

$$V_R \frac{dC}{dt} = -\dot{V}C \rightarrow \frac{dC}{C} = -\frac{dt}{\tau}$$

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

$$E(t) = \frac{C(t)}{\int_0^\infty C(t')dt'} = \frac{C_0 \exp\left(-\frac{t}{\tau}\right)}{C_0\ \tau\,(-\exp(-\infty) + \exp(-0))} = \frac{\exp\left(-\frac{t}{\tau}\right)}{\tau}$$

b) $\bar{t} = \int_0^\infty t' E(t') dt'$

$$\bar{t} = \frac{1}{\tau}\int_0^\infty t' \exp\left(-\frac{t}{\tau}\right) dt'$$

To make our identity appear, let's do a variable change from $t' \rightarrow t'/\tau$

$$\bar{t} = \frac{1}{\tau}\int_0^\infty \tau^2 \, (t'/\tau) \exp\left(-\frac{t'}{\tau}\right) d(t'/\tau) = \frac{\tau^2}{\tau}\int_0^\infty \, (t'/\tau) \exp\left(-\frac{t'}{\tau}\right) d(t'/\tau)$$
$$= \tau \int_0^\infty x \exp(-x) \, d(x) = \tau$$

Which is what we expect…

Problem 2

The equation for an axially dispersed PFR is:

$$\frac{\partial C_i}{\partial \theta} + \frac{\partial C_i}{\partial Z} = \frac{1}{Pe_a}\frac{\partial^2 C_i}{\partial Z^2}$$

For a simple PFR ($Pe_a \rightarrow \infty$), the equation becomes:

$$\frac{\partial C_i}{\partial \theta} + \frac{\partial C_i}{\partial Z} = 0$$

Can you use Laplace transforms to solve this equation and calculate E(t) for a simple dirac (as the input):

$\delta(t) = \infty \; @ \; t = 0 \; and \; \delta(t) = 0 \; for \; t \neq 0$

Reminder: To use Laplace transforms to solve partial differential equations, you should:

1. Transform the equation to Laplace coordinates → this removes time as a variable and results in an ODE (which you know how to solve)
2. Solve the resulting ODE
3. Do the revers Laplace transform to get the final result

Useful Laplace transforms (from Wikipedia):

Useful properties:

	Time domain	s domain	Comment
Linearity	$af(t) + bg(t)$	$aF(s) + bG(s)$	Can be proved using basic rules of integration.
Frequency-domain derivative	$tf(t)$	$-F'(s)$	F' is the first derivative of F.
Frequency-domain general derivative	$t^n f(t)$	$(-1)^n F^{(n)}(s)$	More general form, nth derivative of $F(s)$.
Derivative	$f'(t)$	$sF(s) - f(0)$	f is assumed to be a differentiable function, and its derivative is assumed to be of exponential type. This can then be obtained by integration by parts
Second derivative	$f''(t)$	$s^2F(s) - sf(0) - f'(0)$	f is assumed twice differentiable and the second derivative to be of exponential type. Follows by applying the Differentiation property to $f'(t)$.
General derivative	$f^{(n)}(t)$	$s^nF(s) - \sum_{k=1}^{n} s^{n-k}f^{(k-1)}(0)$	f is assumed to be n-times differentiable, with nth derivative of exponential type. Follows by mathematical induction.

Useful transformations:

Function	Time domain $f(t) = \mathcal{L}^{-1}\{F(s)\}$	Laplace s-domain $F(s) = \mathcal{L}\{f(t)\}$	Region of convergence	Reference
unit impulse	$\delta(t)$	1	all s	inspection
delayed impulse	$\delta(t-\tau)$	$e^{-\tau s}$		time shift of unit impulse
unit step	$u(t)$	$\frac{1}{s}$	$\mathrm{Re}(s) > 0$	integrate unit impulse
delayed unit step	$u(t-\tau)$	$\frac{1}{s}e^{-\tau s}$	$\mathrm{Re}(s) > 0$	time shift of unit step
ramp	$t \cdot u(t)$	$\frac{1}{s^2}$	$\mathrm{Re}(s) > 0$	integrate unit impulse twice
nth power (for integer n)	$t^n \cdot u(t)$	$\frac{n!}{s^{n+1}}$	$\mathrm{Re}(s) > 0$ $(n > -1)$	Integrate unit step n times

Solution:

$$\frac{\partial C_i}{\partial \theta} + \frac{\partial C_i}{\partial Z} = 0$$

Let's apply the Laplace transform:

$$\mathcal{L} \rightarrow S\bar{C} - \bar{C}(Z, \theta = 0) + \frac{d\bar{C}}{dZ} = 0$$

$$\bar{C}(Z, \theta = 0) = 0$$

$$\frac{d\bar{C}}{dZ} = -S\bar{C}$$

$$\frac{d\bar{C}}{\bar{C}} = -SdZ$$

$$\bar{C} = cst \exp(-SZ)$$

We apply the boundary condition:

$$\bar{C}(Z = 0) = \mathcal{L}[C(Z = 0, t)] = \mathcal{L}[\delta(t)] = 1$$

$$@Z = 0,\;\; \bar{C} = cst = 1$$

$$\bar{C} = \exp(-SZ)$$

$$\mathcal{L}^{-1} \rightarrow C = \delta(\theta - Z)$$

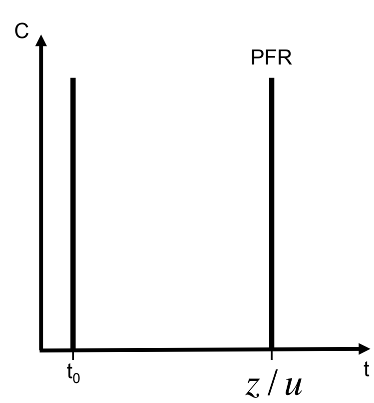
Since:

$$\theta = \frac{t}{\bar{t}} = \frac{tu}{L}$$

$$Z = \frac{z}{L}$$

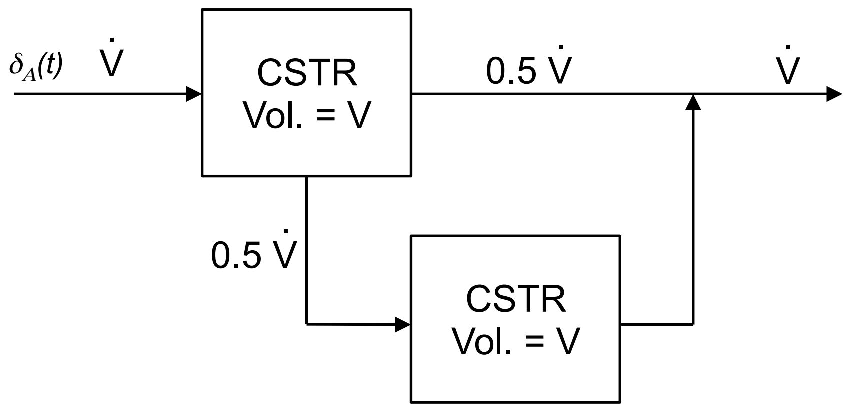
Divide by L/u to get $t - z/u$

$C = \delta(t - z/u)$ with z/u = time spent in the reactor… In other words, it's a dirac delayed by the time spent in the reactor. That's what we expect:



Problem 3

A) Can you find E(t) for the following system? A tracer injection (or dirac, $\delta_A(t)$) was injected at $t=0$ into the following system that contains two CSTRs with equal volume. The initial flowrate is $\dot{V}$ and is split into two after the first CSTR and then mixed back together after the second CSTR.



B) How does it compare to E(t) for a single CSTR of volume 2V?

Solution:

A balance on CSTR 1 yields the following concentration of the tracer as a function of time:

$$C(t) = \frac{n}{\dot{V}} \frac{exp\left(-\frac{t}{\tau}\right)}{\tau}$$

Next, write a balance on CSTR 2:

$$V \frac{dC_{out}}{dt} = 0.5\dot{V}C - 0.5\dot{V}C_{out}$$

Substitute the equation describing $C(t)$:

$$\frac{dC_{out}}{dt} + \frac{0.5}{\tau} C_{out} = \frac{0.5n}{\tau^2 \dot{V}} \exp\left(-\frac{t}{\tau}\right)$$

Solve this first order differential equation (with the initial condition $C_{out}(0) = 0$):

$$C_{out} = \frac{n}{\dot{V}\tau} \exp\left(-\frac{0.5t}{\tau}\right) - \frac{n}{\dot{V}\tau} \exp\left(-\frac{t}{\tau}\right)$$

Write a mass balance at the point where they mix (in = out):

$0.5\dot{V}C + 0.5\dot{V}C_{out} = \dot{V}C_A$

Therefore,

$C_A = 0.5C + 0.5C_{out}$

After substituting equations for $C(t)$ and $C_{out}(t)$, we have:

$$C_A = \frac{n}{2\dot{V}\tau} \exp\left(-\frac{t0.5}{\tau}\right)$$

The RTD, E(t), can be found from the following equation:

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

Therefore,

$$E(t) = \frac{\exp\left(-\frac{0.5t}{\tau}\right)}{2\tau}$$

For a single CSTR with a volume equal to 2V, define
V’=2V

$$\tau' = \frac{2V}{\dot{V}} = 2\tau$$

Therefore, we would have:

$$C(t) = \frac{n}{\dot{V}} \frac{exp\left(-\frac{t}{\tau'}\right)}{\tau'} = \frac{n}{\dot{V}} \frac{exp\left(-\frac{t}{2\tau}\right)}{2\tau}$$

The concentration of a tracer (CA) for a single CSTR with V’=2V is the same as the first system. Therefore, the RTD is also the same.