10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. K. Dane Wittrup
Lecture 10: Non-ideal Reactor Mixing Patterns

This lecture covers residence time distribution (RTD), the tanks in series model, and combinations of ideal reactors.

Non-Ideal Mixing

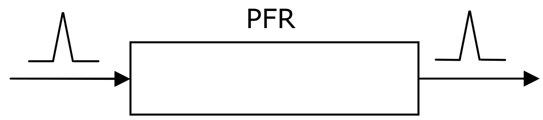

Figure 1. Ideal PFR with pulse input. A pulse input will yield an output profile that is a pulse input.

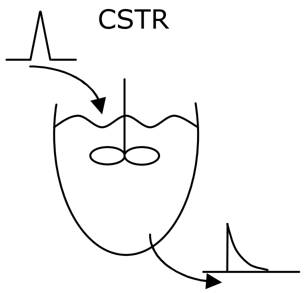

Figure 2. Ideal CSTR with pulse input. A pulse input will yield an output profile that is a sharp peak with a tail.

Real mixed tank

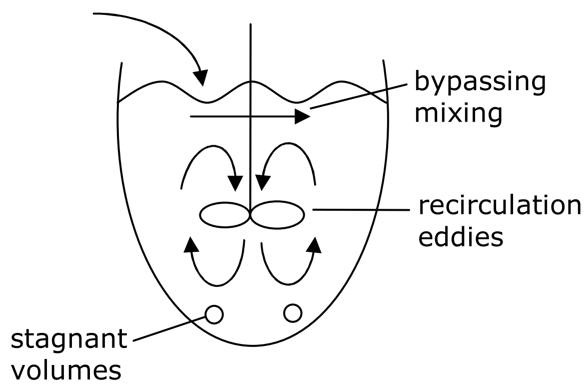

Figure 3. A real mixed tank. In a real mixed tank there are portions that are not well mixed due to stagnant volumes, recirculation eddies, and mixing bypasses.

In a real PFR there is back-mixing and axial dispersion. In a packed bed reactor (PBR) channeling can occur. This is where the fluid channels through the solid medium.

Residence Time Distribution

A useful diagnostic tool is the residence time distribution (RTD). The residence time is how long a particle stays in the reactor once entering.

$E(t)\,dt \equiv$ Probability that a fluid element entering the vessel at t=0 exits between time t and t+dt.

Probability density function for exit time, t, as a random variable.

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$\int_0^t E(t)\,dt$ Probability that fluid element exits before time t.

$\int_t^\infty E(t)\,dt$ Probability of exiting at time later than t.

mean t $= \int_0^\infty tE(t)\,dt = \tau$

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

variance $= \sigma^2 = \int_0^\infty (t-\tau)^2 E(t)\,dt$ (measures the broadness of the distribution)

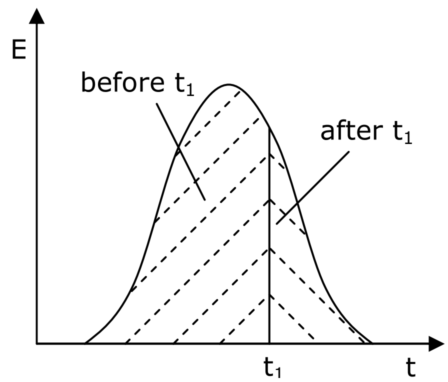

Figure 4. E(t) versus t. At a given time point, some material has exited and some material will still exit at a later time.

Experimental Determination of E(t)

Inflow should be something measurable
-Absorbance
-Fluorescence
-pH
-salt-conductivity
-radioactivity

Use one of two types of input concentration curves:

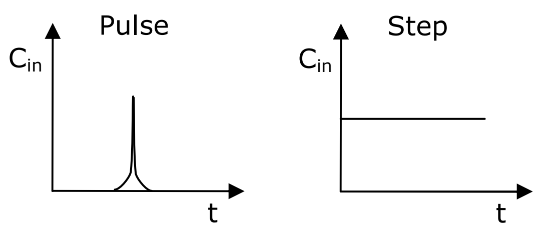

Figure 5. Two types of input. A pulse input is a spike of infinite height but zero width, ideally. A step input is a constant concentration over a period of time.

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A pulse input allows for easy interpretation because all materials enter the reactor at once.

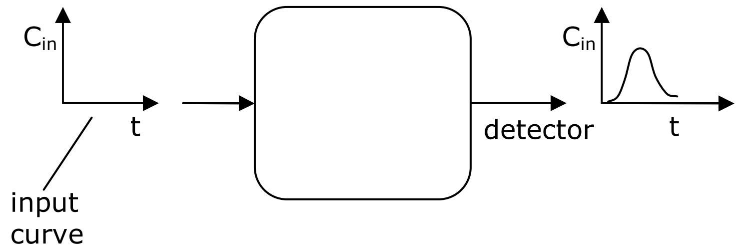

Figure 6. Schematic of a residence-time distribution experiment. The input curve enters the reactor; a detector detects concentration changes in the output stream.

$$E(t)=\frac{C_{out}(t)}{\int_0^t C_{out}(t)\,dt}$$

PFR (Ideal)

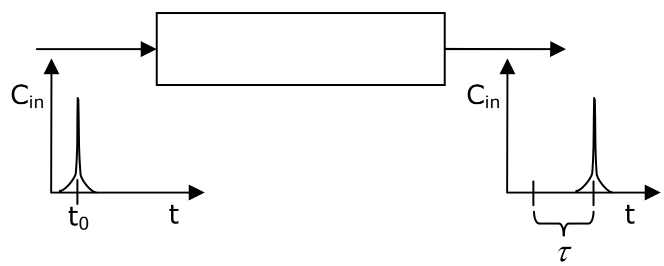

Figure 7. Pulse input in ideal PFR. A pulse input in an ideal PFR becomes a pulse output.

$$E(t)=\delta(t-\tau)$$

$$\delta(x)=\begin{cases}=0 & x\neq 0\\ =\infty & x=0\end{cases}$$

$$\int_{-\infty}^{\infty}\delta(x)\,dx=1$$

$$\int_{-\infty}^{\infty}f(x)\,\delta(x-a)\,dx=f(a)$$

CSTR (Ideal)

Transient material balance:
In-Out+Production=Accumulation

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Since all the material is added at once, In=0. The tracer used is non-reactive. Therefore there is no production. This gives:

$$0 - v_0 C + 0 = V \frac{dC}{dt}$$

$$C(t) = C_0 e^{-t/\tau}, \quad \tau = \frac{V}{v_0}$$

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt} = \frac{e^{-t/\tau}}{\tau}$$

CSTR

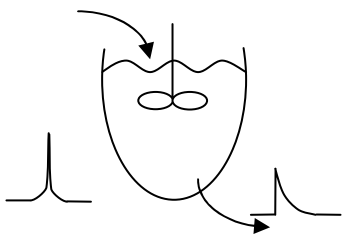

Figure 8. Pulse input in an ideal CSTR. In an ideal CSTR, a pulse input leads to a sharp peak with a tail.

$$\text{mean residence time} = \int_0^\infty \frac{t e^{-t/\tau}}{\tau} dt = \tau$$

CSTR (non-ideal mixing)

Bypassing: Divide input into 2 streams

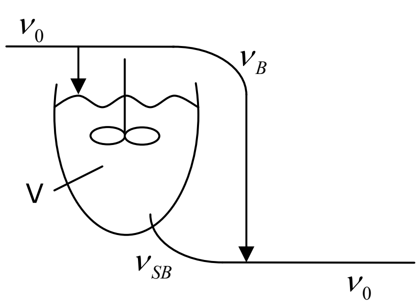

Figure 9. A bypass is modeled by dividing the input stream into two streams, one of which does not enter the reactor.

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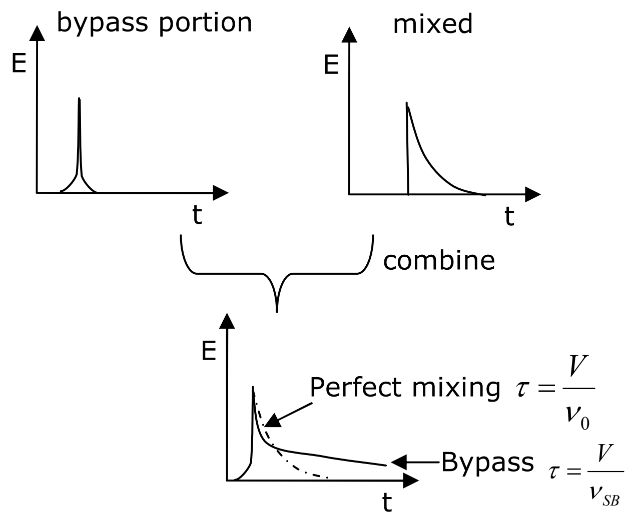

Figure 10. Residence-time distribution determination for a bypass.

Dead volumes: Stagnant regions not getting mixed

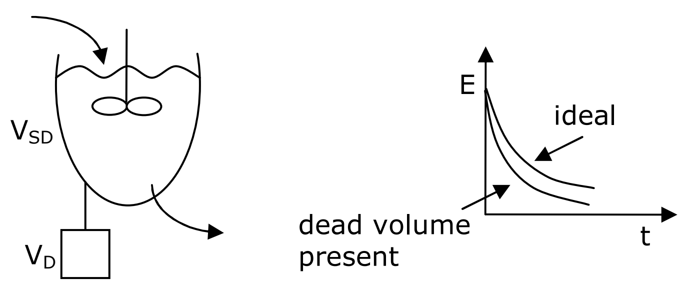

Figure 11. Residence-time distribution for dead volumes**.** When a dead volume is present, a decreased amount of material is observed in the output stream.

measureable $V=V_{SD}+ V_D$

$$\tau_{SD} = \frac{V_{SD}}{v_0} < \tau_{ideal}$$

PFR (Non-ideal)

Channeling

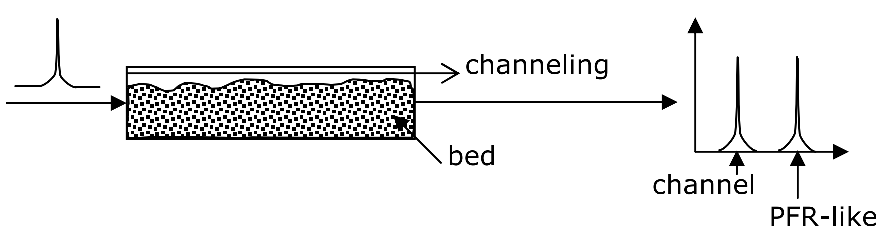

Figure 12. Channeling. In channeling, the residence-time distribution will show peaks for each channel as well as the one for the main portion of the reactor.

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Axial Dispersion

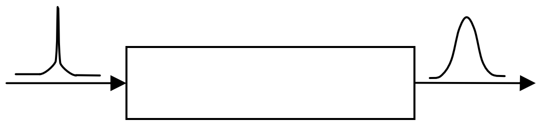

Figure 13. A pulse input can become an axially dispersed pulse output in a non-ideal PFR.

There are two common models for dispersion in a tubular reactor:
-Tanks in a series
-Taylor dispersion model (based on the Peclet number)

To model the PFR as several tanks in a series, break the reactor volume, V, into n CSTRs of volume $\frac{V}{n}$ each.

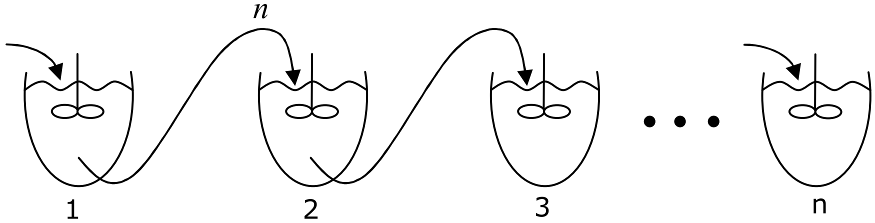

Figure 14. n tanks in series. The output of tank 1 is the input to tank 2. The output is sampled at tank n for dispersion.

$$E(t)=\frac{t^{n-1}}{(n-1)!\tau_i^n}e^{-t/\tau_i}\ ,\ \tau_i=\frac{\tau}{n}$$

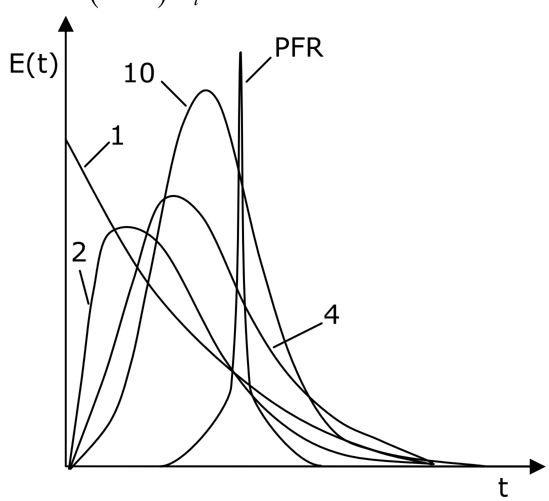

Figure 15. E(t) plots for 1, 2, 4, and 10 tanks and a PFR. Notice how the E(t) curve approaches the PFR pulse as more tanks are used.

The numbers above represent numbers of CSTRs. Without enough CSTRs, the peak is not a good approximation to the narrow peak for a PFR when there is a pulse input.

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$$\sigma^2 = \frac{\tau^2}{n}$$

$$n = \frac{\tau^2}{\sigma^2}$$

We can physically measure τ and we can determine σ from experimentally measuring E(t).

RTD (residence time distribution) are useful for diagnosis, but not for reactor design.

To calculate conversion, the most straightforward tactic is to model the non-ideal system as compartmental combinations of ideal reactors.

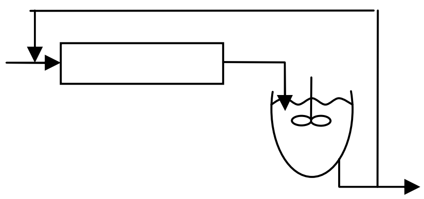

Figure 16. Recirculation. Recirculation can be modeled by a PFR followed by a CSTR with a recycle stream.

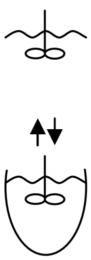

Figure 17. Partially dead volumes. Dead volumes can be modeled as separate CSTRs that exchange material with each other.

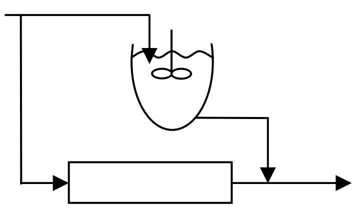

Figure 18. Bypass. A bypass can be modeled as a CSTR along one route with a PFR along the bypass route.

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