

3.044 Problem Set 6

Continuous Flow Reactors

Solutions

1. Batch and continuous flow reactors

- (a) The productivity of continuous flow reactors, as defined in this problem, may be evaluated by solving the conversion expressions for Q . In plug flow, this gives:

$$\frac{C_{A,out}}{C_{A,in}} = \exp\left(-\frac{kV}{Q}\right)$$

$$Q = -\frac{kV}{\ln \frac{C_{A,out}}{C_{A,in}}}$$

And for perfect mixing/CSTR:

$$\frac{C_{A,out}}{C_{A,in}} = \frac{1}{1 + \frac{kV}{Q}}$$

$$1 + \frac{kV}{Q} = \frac{C_{A,in}}{C_{A,out}}$$

$$Q = \frac{kV}{\frac{C_{A,in}}{C_{A,out}} - 1}$$

- (b) For the batch reactor with downtime t_d and residence time t_R , the productivity is the volume divided by the total time $V/(t_R + t_d)$. The residence time can be determined from the batch conversion equation:

$$\frac{C_{A,out}}{C_{A,in}} = e^{-kt_R}$$

$$t_R = -\frac{1}{k} \ln \frac{C_{A,out}}{C_{A,in}}$$

The productivity is then:

$$"Q" = \frac{V}{t_R + t_d} = \frac{V}{-\frac{1}{k} \ln \frac{C_{A,out}}{C_{A,in}} + t_d} = \frac{kV}{-\ln \frac{C_{A,out}}{C_{A,in}} + kt_d}$$

In the limit where t_d/t_R goes to zero, the second term in the denominator vanishes and this approaches the productivity of the plug flow reactor.

Another way to express this is:

$$"Q" = \frac{V}{t_R + t_d} = \frac{V}{t_R} \frac{t_R}{t_R + t_d} = -\frac{kV}{\ln \frac{C_{A,out}}{C_{A,in}}} \frac{t_R}{t_R + t_d}$$

This is fine, but since t_R is a dependent variable, putting it on the right side does not allow direct calculation of the productivity from reactor characteristics as can be done with the expression above.

(c) In this case with a target $C_{A,out}/C_{A,in} = 0.05$, the plug flow reactor's productivity is:

$$Q = -\frac{kV}{\ln 0.05} = \frac{kV}{3.0}$$

And for perfect mixing/CSTR:

$$Q = \frac{kV}{\frac{1}{0.05} - 1} = \frac{kV}{19}$$

For a batch reactor:

$$"Q" = \frac{kV}{-\ln \frac{C_{A,out}}{C_{A,in}} + kt_d} = \frac{kV}{3.0 + kt_d}$$

The plug flow reactor is clearly $\frac{1/3}{1/19} = 6.34$ times more productive than the perfect mixing reactor. And since h_D , A , V and t_d are all positive, the batch reactor will have slightly lower productivity than the plug flow reactor as well, with the ratio depending on the downtime.

(d) The perfect mixing reactor is likely to give the highest quality output for a couple of reasons:

- In the batch reactor, significant concentration inhomogeneities can develop, particularly if k is temperature-dependent and the reaction gives off or consumes a significant amount of heat (much more so in a heterogeneous/surface reactor). Reactions with the containment vessel will also introduce location-dependent variations in composition. For these reasons, it's often desirable to stir a batch reactor.
- A plug flow reactor will always exhibit significant concentration inhomogeneities longitudinally, and sometimes across the reactor for the same reason as the batch reactor. If flow conditions or input concentrations deviate at all from steady state, changes in flow patterns can result in inhomogeneity in the output.
- If the raw material in a plug flow reactor enters at varying concentration, that variation will carry through to the end of the reactor, and show up as inhomogeneous output. A perfect mixing reactor, on the other hand, will rapidly mix in any concentration departures in the raw material, smoothing out their influence over time.

(e) Batch reactors have several advantages over continuous flow reactors:

- They can be stopped between batches, so the production rate is flexible and can be varied if economically desirable. If a continuous reactor is stopped, it takes time and wastes material to return it to consistent steady-state production.
- Batch reactors are also more flexible, in that one can easily use different compositions in different batches to produce products with different specifications.
- If the process degrades the reactor in some way, a batch reactor can be cleaned, relined, etc. between batches, where continuous reactors must run for a long time before that can be done.
- Because flaws tend to be isolated to a given batch, one can track the quality more easily in a batch process. For example, when the cause of a plane is traced to a flaw in a titanium part, it is common practice to ground all planes with parts made from the same vacuum arc remelt (VAR) titanium ingot, and other defective parts are often found in the subsequent inspections.
- If the reactants are stirred, a batch reactor can often achieve better quality than a plug flow reactor (which cannot be well-mixed in order to maintain plug flow), and better productivity than a continuous flow reactor (as seen above).

Any of the above receives full credit.

2. Evaporation of volatile impurities during electron beam melting

All numerical answers are in the table at the end.

(a) For plug flow:

$$\frac{C_{out}}{C_{in}} = \exp\left(-\frac{k''A}{Q}\right)$$

(b) For perfect mixing:

$$\frac{C_{out}}{C_{in}} = \frac{1}{1 + \frac{k''A}{Q}}$$

(c) Even if the hearth is well-mixed, assuming unit activity coefficients, vacuum hearth melting is very effective at removing lead, cadmium and zinc impurities from titanium.

Element	\bar{p}_v , torr	J_{ev} , $\frac{\text{mol}}{\text{m}^2 \cdot \text{s}}$	k'' , $\frac{\text{m}}{\text{s}}$	Plug $\frac{C_{in}}{C_{out}}$	Mixing $\frac{C_{in}}{C_{out}}$
Cd	1.81×10^5	2.21×10^5	2.59	8×10^{-12771}	3.40×10^{-5}
Pb	787	709	8.29×10^{-3}	1.3×10^{-41}	1.05×10^{-2}
Zn	9.56×10^4	1.53×10^5	1.79	6.3×10^{-8837}	4.91×10^{-5}

3. Flow through a catalytic reactor

(a) This is a straightforward application of tube bundle theory equations:

$$R_h = \frac{V_h}{A_w} = \frac{\omega}{S_0(1-\omega)}$$

Pore fraction ω is given as 0.4, and S_0 is the ratio of surface area to solid volume which for a bunch of monodisperse (uniform size) spheres is:

$$S_0 = \frac{4\pi R^2}{\frac{4}{3}\pi R^3} = \frac{3}{R}$$

With these parameters, the hydraulic radius becomes:

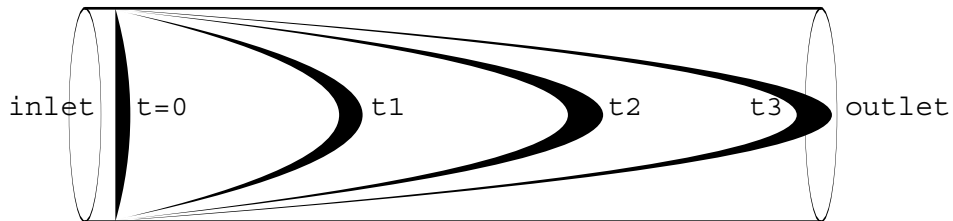
$$R_h = \frac{0.4}{\frac{3}{1\text{mm}}(1-0.4)} = 0.22\text{mm},$$

and the specific permeability is:

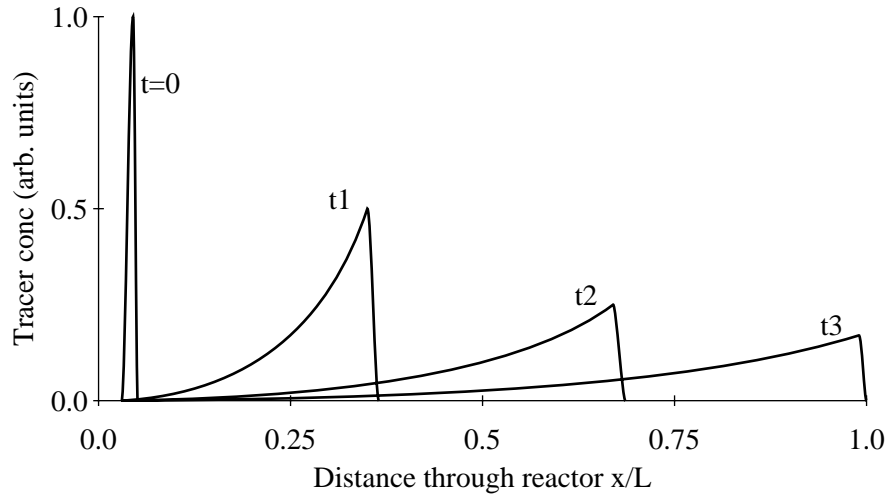
$$\mathcal{P} = K_1 \frac{\omega^3}{S_0^2(1-\omega)^2} = \frac{1}{4.2} \frac{0.4^3}{\left(\frac{3}{1\text{mm}}\right)^2 (1-0.4)^2} = 0.0047\text{mm}^2 = 4.7 \times 10^{-9}\text{m}^2.$$

(b) If the actual permeability is $2.1 \times 10^{-8}\text{m}^2$, this is likely because of the porosity of the spheres themselves, given the diagram of a typical porous sphere.

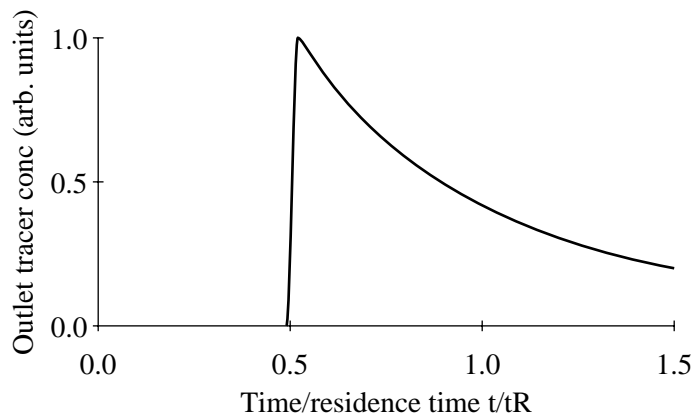
(c) This is a bit complicated, and depends on the profile with which the tracer is injected. As a first approximation, since we're thinking of this as a bundle of tubes, assume that it follows the fluid flowing through a tube, that is, the tracer distributed according to the velocities with more in the center and less on the sides. The tracer distribution across a tube at several times would thus look something like:



With the bulk of the tracer in the center of the tube, the average concentration vs. distance from the entrance at several times would look like:



The first bit of tracer reaches the outlet at the maximum velocity, which in a tube is twice the average velocity, so the time will be half of the average residence time. The outlet tracer concentration vs. time will thus look something like:



- (d) A long lead time before the first tracer arrives indicates poor mixing. That a lot of tracer arrives all at once sounds something like a “plug”. And a relatively narrow approximate L'_D (width of the distribution, see second figure in part 3c above) when the first tracer arrives indicates that plug flow is a good candidate for the reactor behavior.

On the other hand, that the first tracer reaches the end in half of the average residence time means that there is some “mixing” going on due to the non-uniform velocity. So actual behavior will not exactly follow plug flow, it will fall somewhere between that and perfect mixing, but closer to plug flow.