

# **Compartment Models**

## **Chapter 12**

- This chapter are the next stage beyond the very simplest, those that assume the extremes of plug flow and mixed flow.
- In the compartment models we consider the vessel and the flow through it as follows:

$$\text{Total volume } \cdot \cdot \cdot \left\{ \begin{array}{l} V_p \text{—plug flow region} \\ V_m \text{—mixed flow region} \\ V_d \text{—dead or stagnant region within the vessel} \end{array} \right\} V_a \text{—active volume}$$

$V$

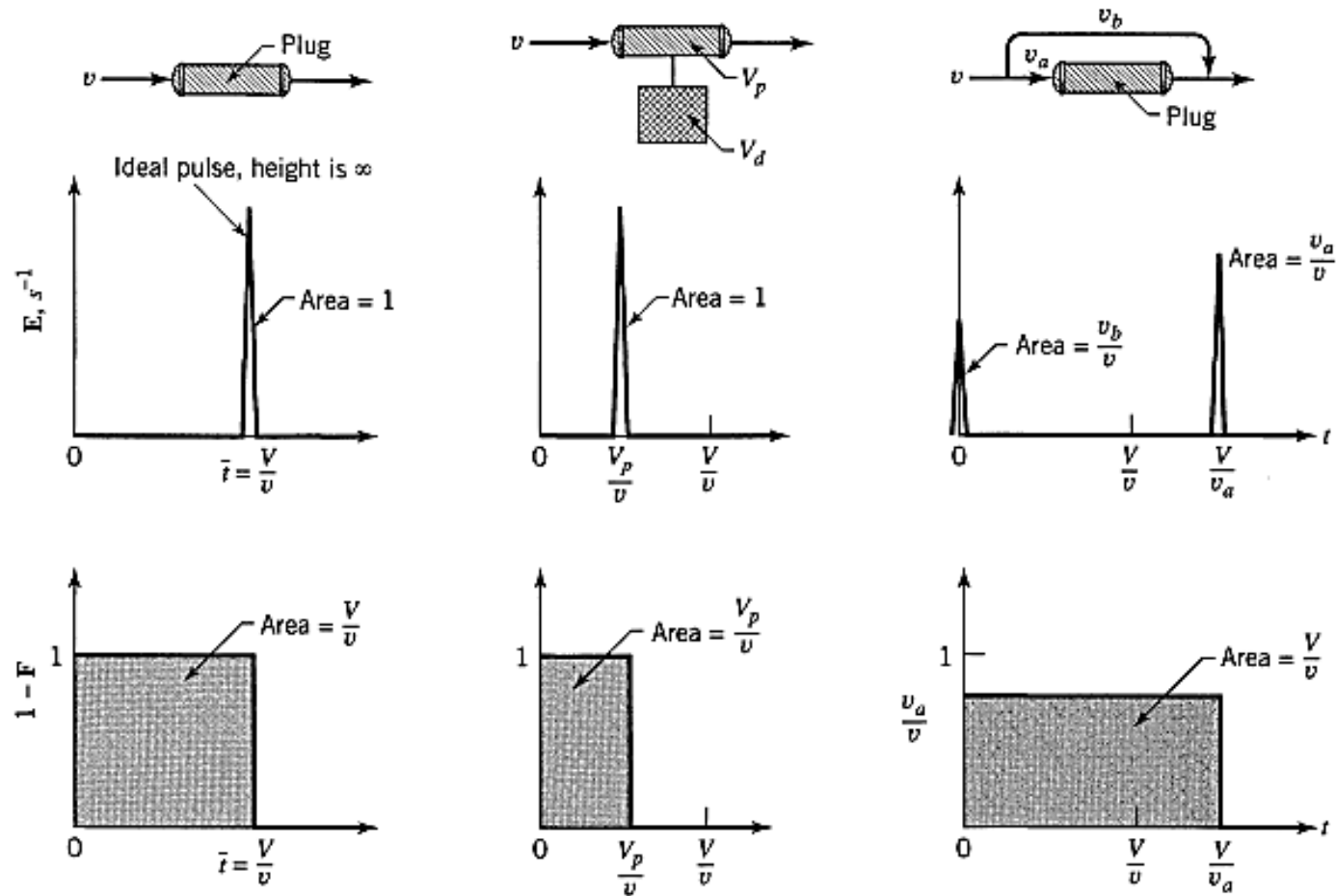
$$\text{Total throughflow } \cdot \cdot \cdot \left\{ \begin{array}{l} v_a \text{—active flow, that through the plug and mixed flow regions} \\ v_b \text{—bypass flow} \\ v_r \text{—recycle flow} \end{array} \right.$$

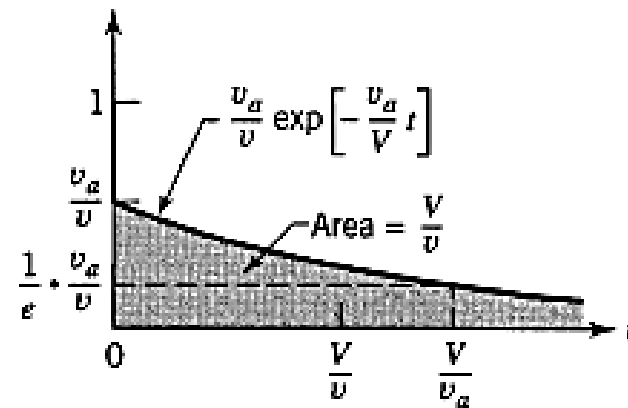
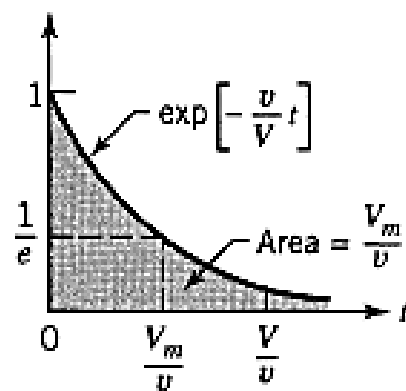
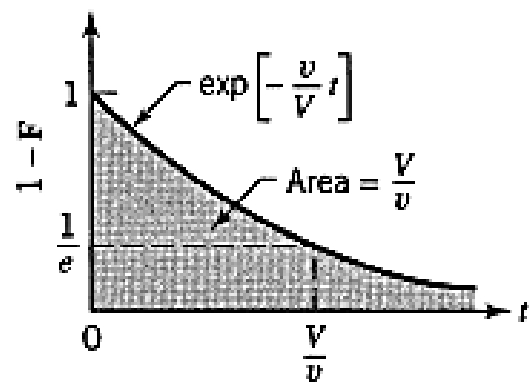
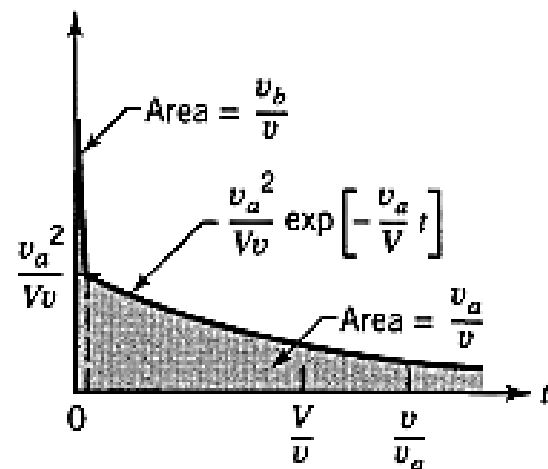
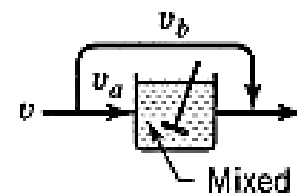
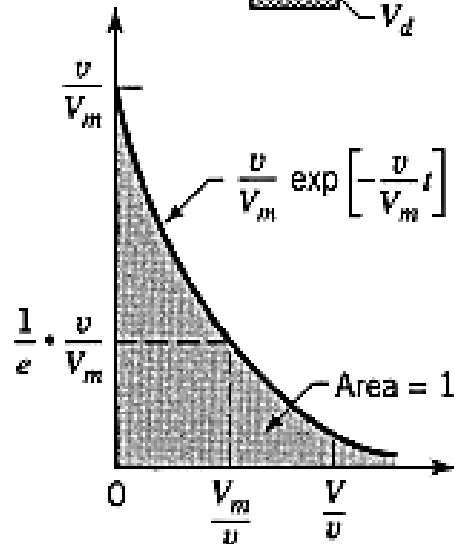
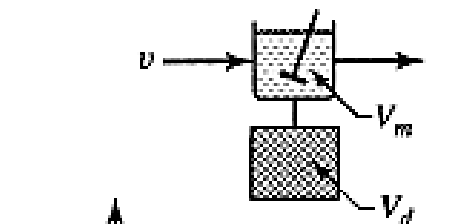
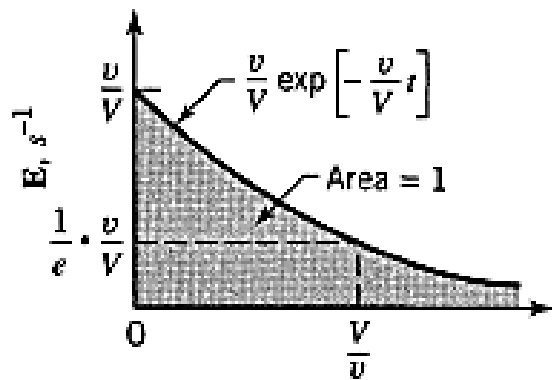
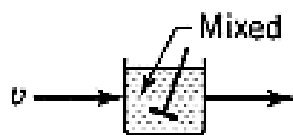
$v$

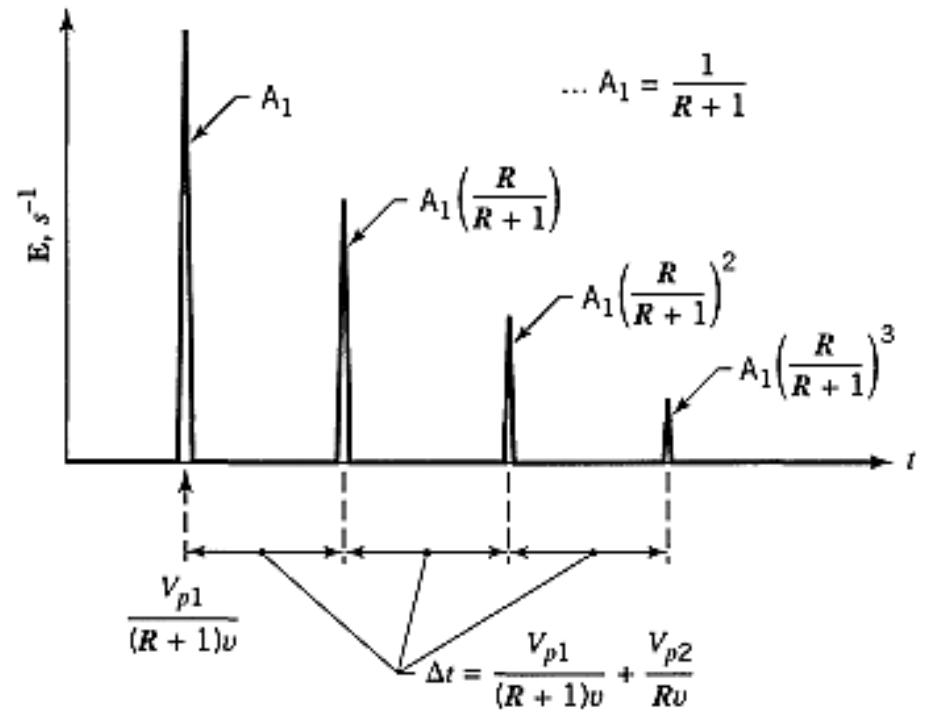
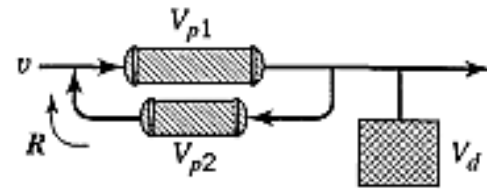
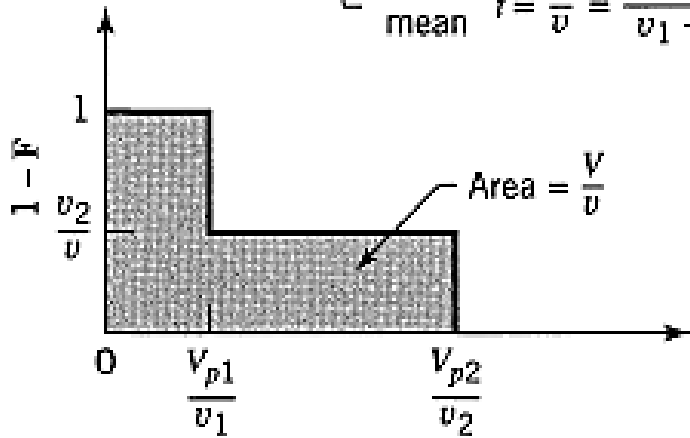
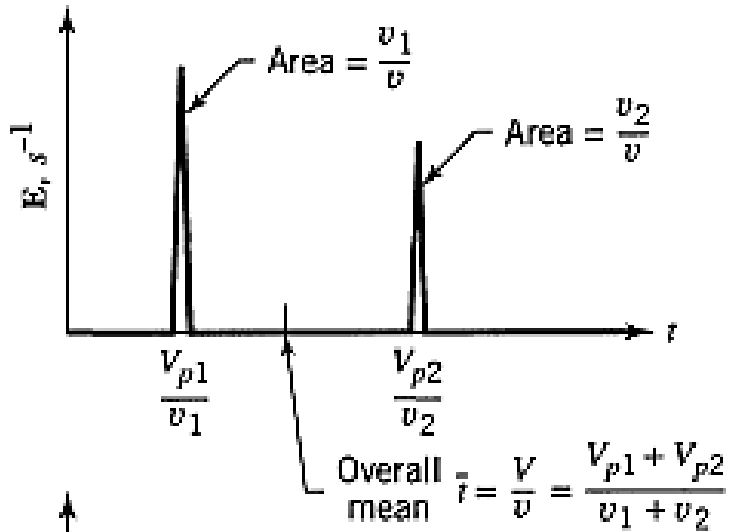
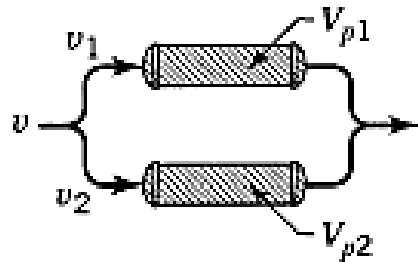
By comparing the E curve for the real vessel with the theoretical curves for various combinations of compartments and through flow, we can find which model best fits the real vessel.

Of course, the fit will not be perfect; however, models of this kind are often a reasonable approximation to the real vessel.

- Figure, shows what the E curves look like for various combinations of the above elements-certainly not all combinations.







# Hints, Suggestions, and Possible Applications

(a) If we know  $M$  (kilograms of tracer introduced in the pulse) we can make a material balance check.

Remember that  $M = v$  (area of curve).

However, if we only measure the output  $C$  on an arbitrary scale, we cannot find  $M$  or make this material balance check.

(b) We must know both  $V$  and  $v$  if we want to properly evaluate all the elements of a model, including dead spaces. If we only measure jobs, we cannot find the size of these stagnant regions and must ignore them in our model building.

Thus

If the real vessel  
has dead spaces:

$$\bar{t}_{\text{obs}} < \bar{t}$$

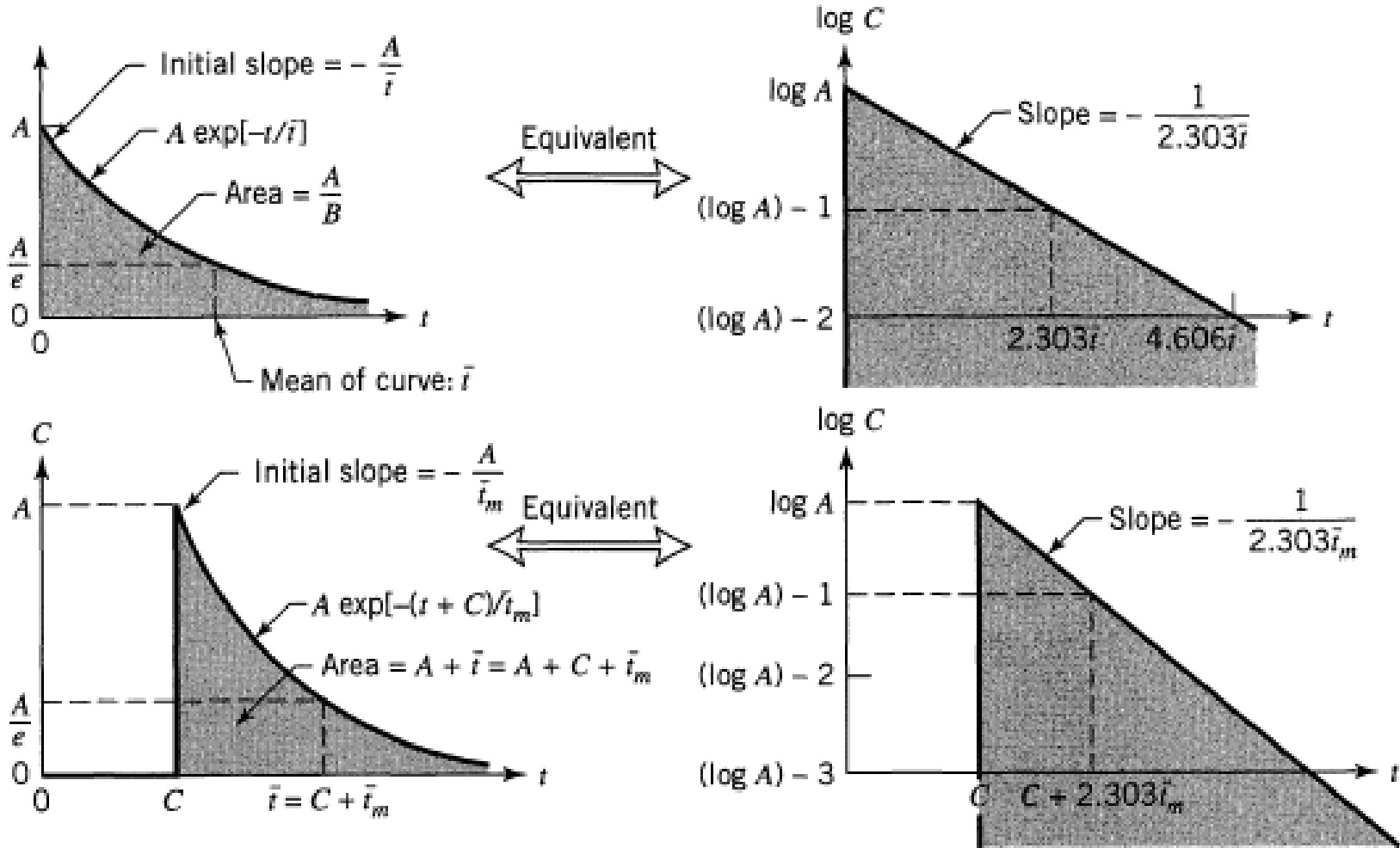
If the real vessel  
has no dead spaces:

$$\bar{t}_{\text{obs}} = \bar{t}$$

$$\dots \text{ where } \begin{cases} \bar{t} = \frac{V}{v} \\ \bar{t}_{\text{obs}} = \frac{V_{\text{active}}}{v} \end{cases}$$

(c) The semilog plot is a convenient tool for evaluating the flow parameters of a mixed flow compartment.

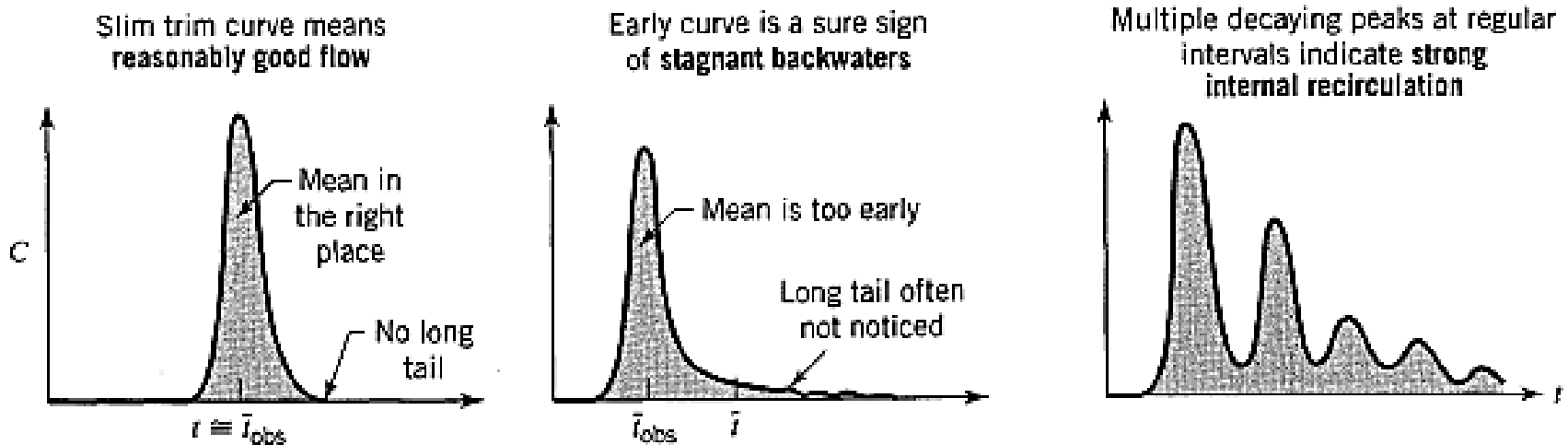
Just draw the tracer response curve on this plot, find the slope and intercept and this gives the quantities **A**, **B**, and **C**, as shown in Fig.



# Diagnosing Reactor IIs

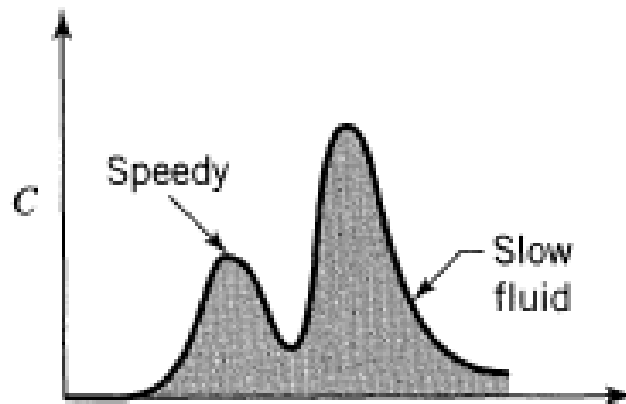
- These combined models are useful for diagnostic purposes, to pinpoint faulty flow and suggest causes.
- For example, if you expect plug flow and you know  $\bar{t} = V/v$ ,

Fig. shows what you could find. If you expect mixed flow, Fig. shows what you may find.

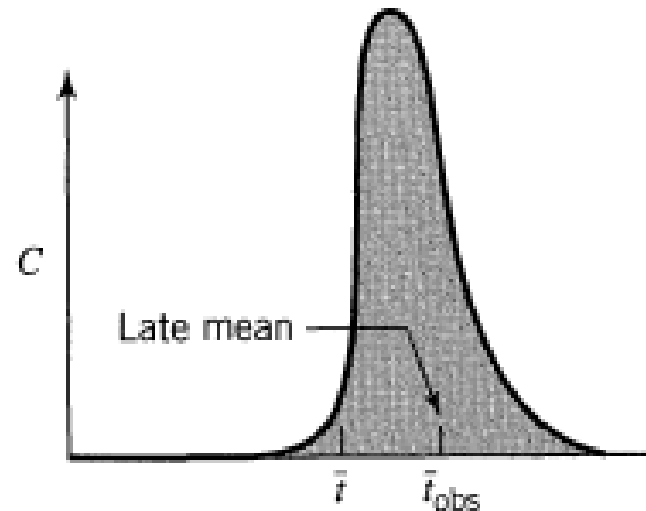




Double peaks come from flow in parallel paths, channeling

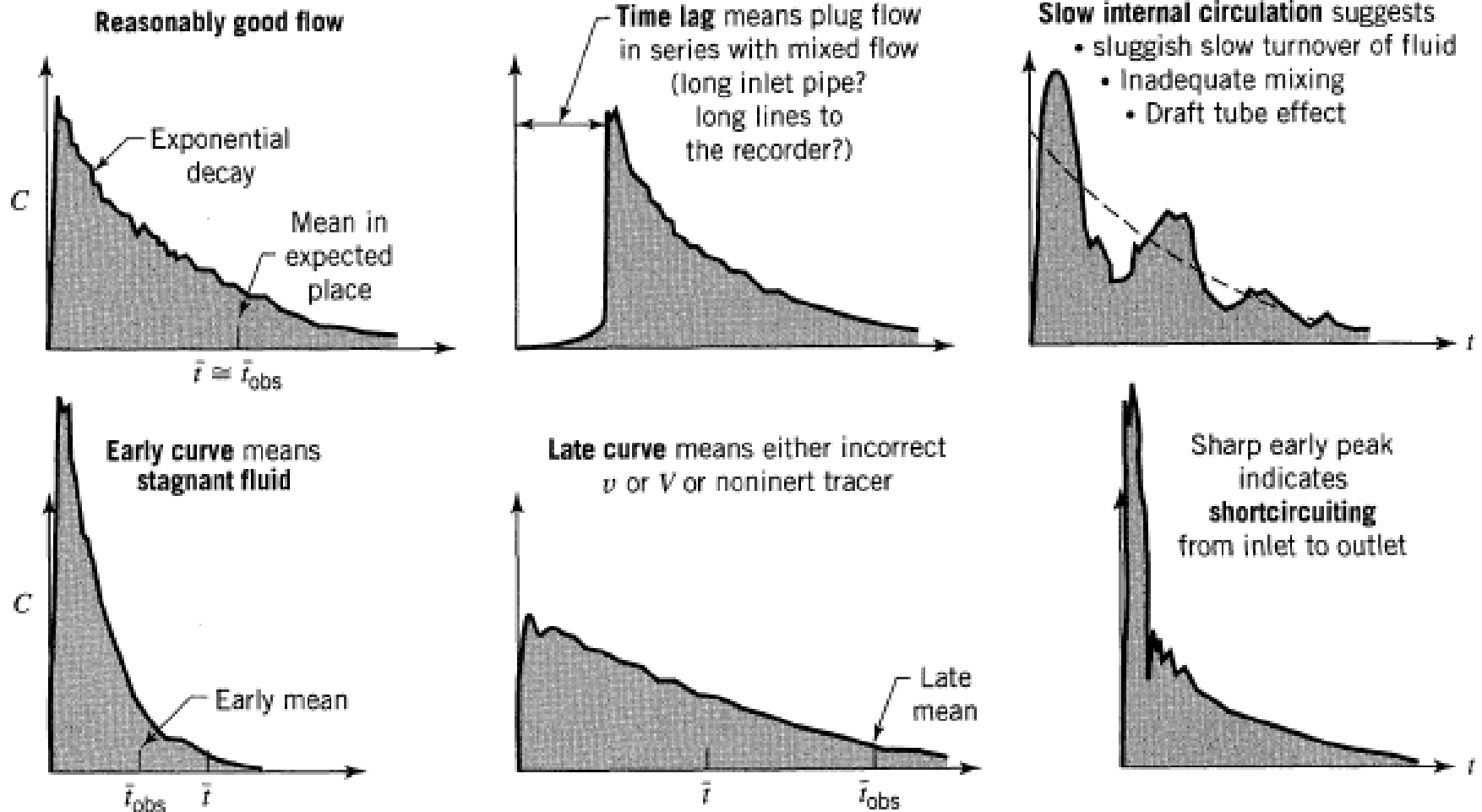


Late curve



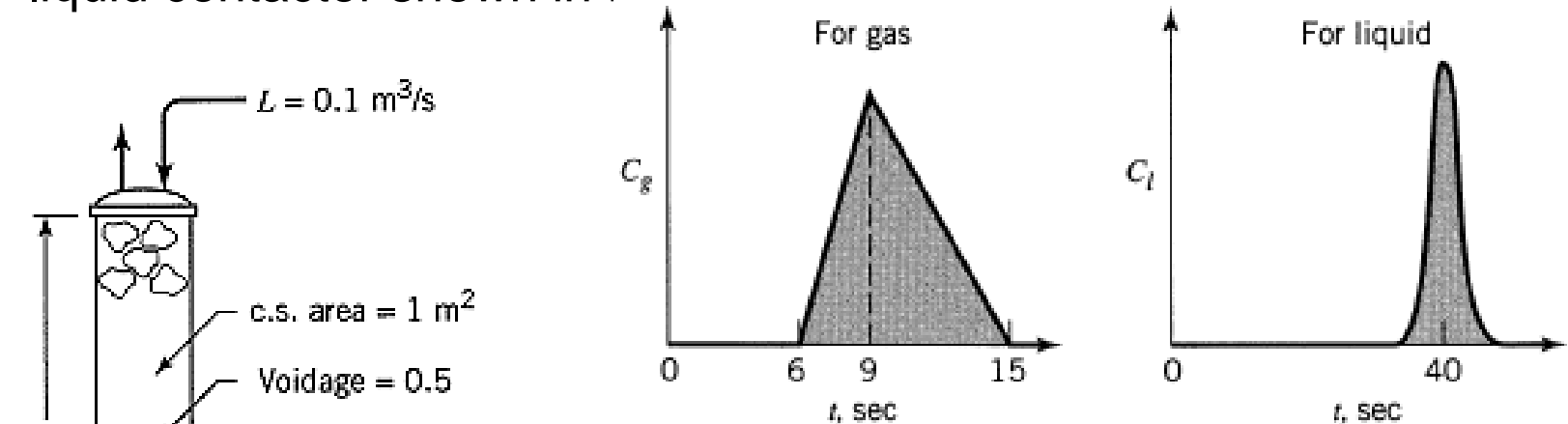
Late tracer is puzzling. Material balance says it can't happen so the only explanations are:  $v$  or  $V$  are incorrectly measured (check flow meters)  
tracer is not inert (adsorbs on surface? Try a different one)  
the closed vessel assumption is far from satisfied.

- If you expect mixed flow, Fig. shows what you may find.



# BEHAVIOR OF A G/L CONTACTOR

- From the measured pulse tracer response curves (see figure), find the fraction of gas, of flowing liquid, and of stagnant liquid in the gas-liquid contactor shown in |



To find  $V_g$ ,  $V_l$ , and  $V_{\text{stag}}$ , first calculate  $\bar{t}_g$  and  $\bar{t}_l$  from the tracer curves.

$$\bar{t}_g = \frac{\sum tC}{\sum C} = \frac{8(9-6)(h/2) + 11(15-9)(h/2)}{(15-6)(h/2)} = 10 \text{ s}$$

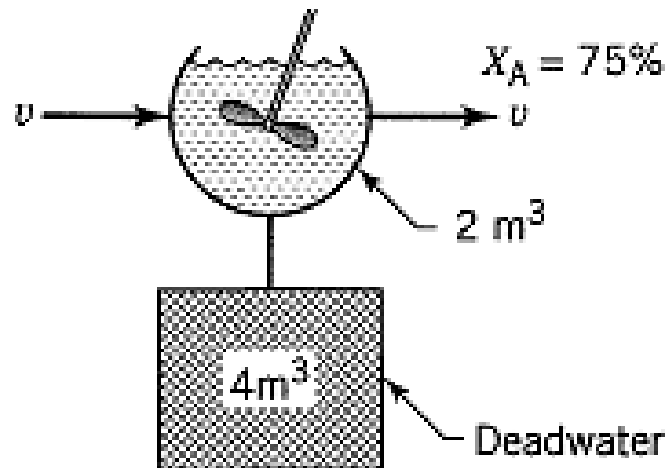
$$\bar{t}_l = 40 \text{ s.} \quad V_g = \bar{t}_g v_g = (10)(0.5) = 5 \text{ m}^3$$

$$V_l = \bar{t}_l v_l = 40(0.1) = 4 \text{ m}^3$$

$$\left. \begin{array}{l} \% G = 50\% \\ \% L = 40\% \\ \% \text{ stagnant} = 10\% \end{array} \right\} \leftarrow$$

## CURING A MISBEHAVING REACTOR

At present our 6-m<sup>3</sup> tank reactor gives 75% conversion for the first order reaction  $A \rightarrow R$ . However, since the reactor is stirred with an underpowered paddle turbine, we suspect incomplete mixing and poor flow patterns in the vessel. A pulse tracer shows that this is so and gives the flow model sketched in Fig. E12.2. What conversion can we expect if we replace the stirrer with one powerful enough to ensure mixed flow?



Let subscript 1 represent today's reactor and subscript 2 represent the cured reactor.

At present, for the MFR, we have

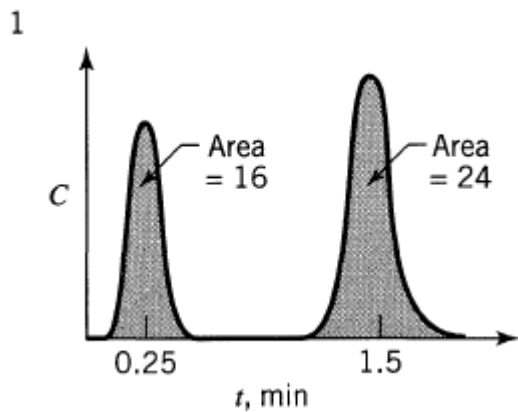
$$k\tau = \frac{C_{A0} - C_A}{C_A} = \frac{C_{A0}}{C_A} - 1 = \frac{1}{0.25} - 1 = 3$$

$$\text{But } k\tau_2 = 3 k\tau_1 = 3 \times 3 = 9$$

$$\frac{C_{A2}}{C_{A0}} = \frac{1}{k\tau_2 + 1} = \frac{1}{9 + 1} = 0.1$$

$$X_{A2} = \underline{90\%}$$

**12.1. to 12.6.** A pulse of concentrated NaCl solution is introduced as tracer into the fluid entering a vessel ( $V = 1 \text{ m}^3$ ,  $v = 1 \text{ m}^3/\text{min}$ ) and the concentration of tracer is measured in the fluid leaving the vessel. Develop a flow model to represent the vessel from the tracer output data sketched in Figs. P12.1 to P12.6.



12.1

This looks like two plug flow units side by side. from fig 1 with

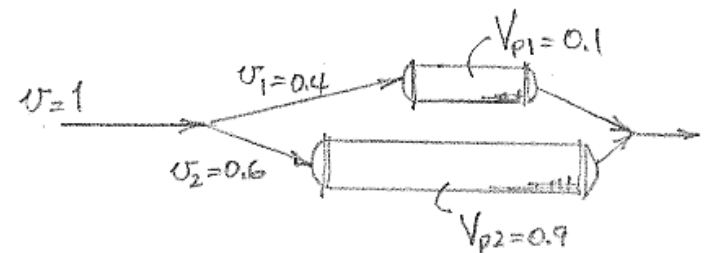
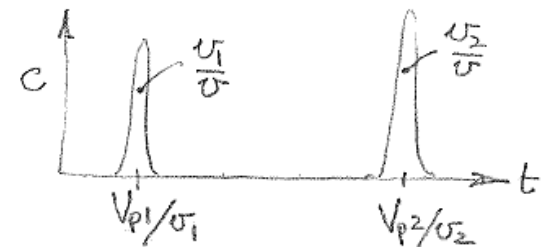
$V_{\text{total}} = 1 \text{ m}^3$  and  $v = 1 \text{ m}^3/\text{s}$  we have

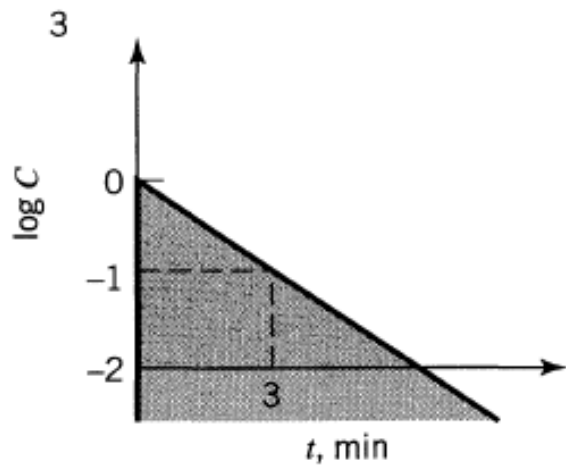
$$v_1 = \frac{16}{16+24} = 0.4 \text{ m}^3/\text{min}$$

$$v_2 = \frac{24}{16+24} = 0.6 \text{ m}^3/\text{min}$$

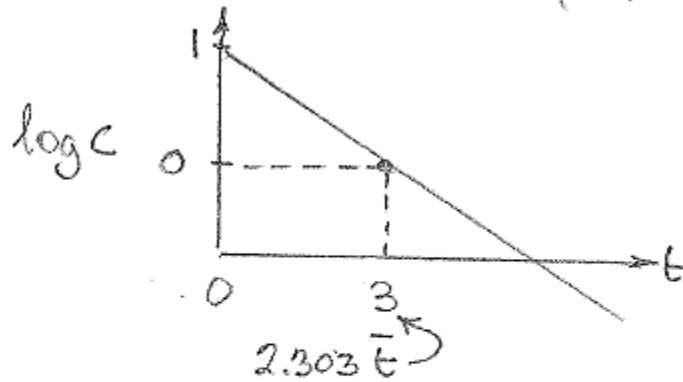
$$V_{p1} = \bar{t}_1 v_1 = (0.25)(0.4) = 0.1 \text{ m}^3$$

$$V_{p2} = \bar{t}_2 v_2 = (1.5)(0.6) = 0.9 \text{ m}^3$$





This looks like a mixed flow unit. Look at Fig. 2



Here  $2.303 \bar{t} = 3$   
 or  $\bar{t} = 1.3 \text{ min}$  } from experiment

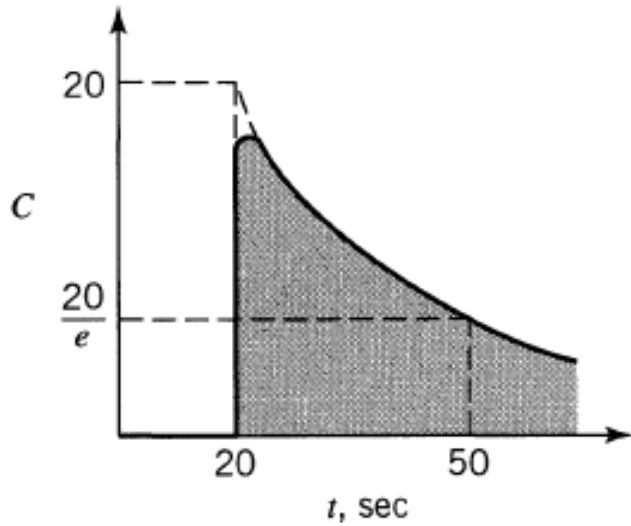
But we know that

$$\bar{t} = \frac{V}{\sigma} = \frac{1 \text{ m}^3}{1 \text{ m}^3/\text{min}} = 1 \text{ min}$$

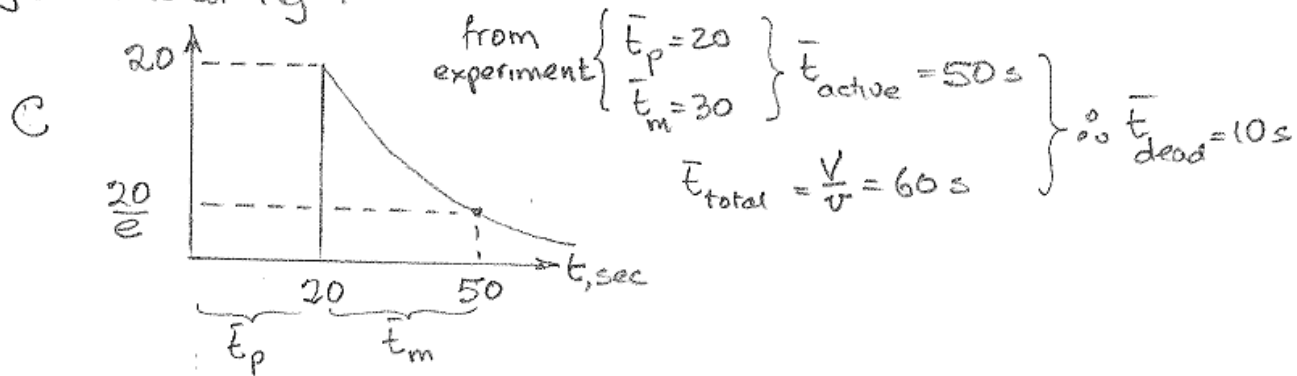
or less if there is dead space

What does this mean? Either the tracer used is not a proper tracer - denser than the fluid, adsorbs on the walls of the vessel, etc - or something else is wrong. Check the experiment

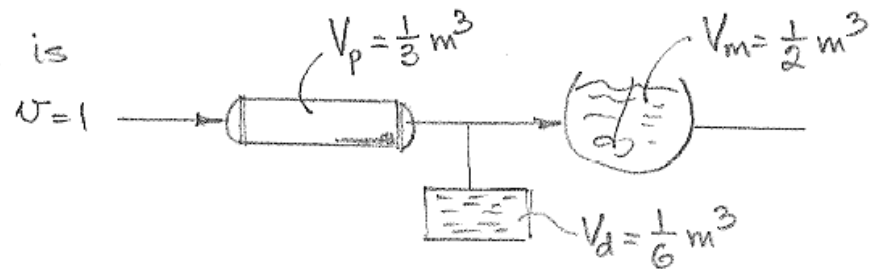
5



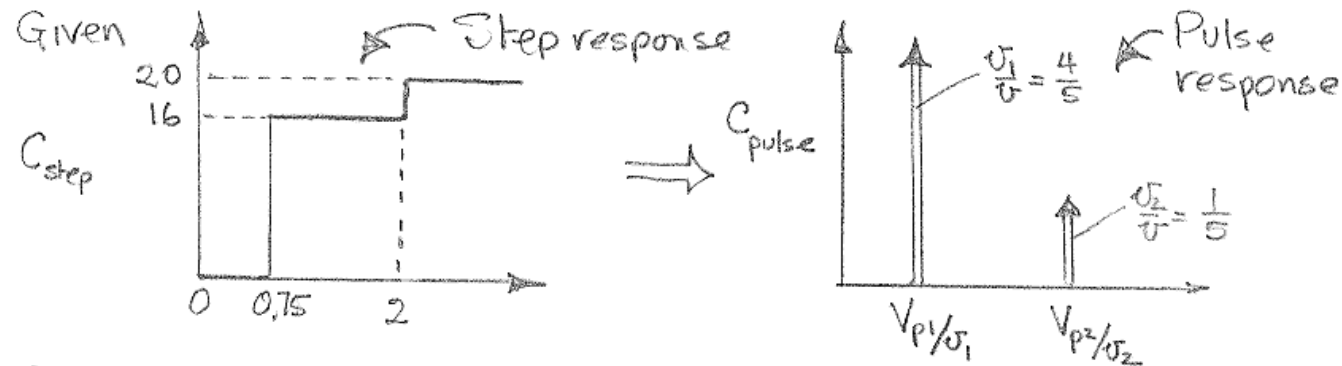
Again look at Fig 1



Thus our model is



**12.7. to 12.10.** A step input tracer test (switching from tap water to salt water, measuring the conductivity of fluid leaving the vessel) is used to explore the flow pattern of fluid through the vessel ( $V = 1 \text{ m}^3$ ,  $v = 1 \text{ m}^3/\text{min}$ ). Devise a flow model to represent the vessel from the data of Figs. P12.7 to P12.10.



From the pulse response curve

$$U_1 = \frac{4}{5} U = 0.8$$

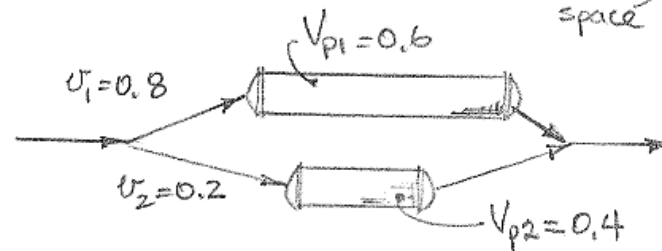
$$U_2 = \frac{1}{5} U = 0.2$$

$$V_{p1} = U_1(0.75) = 0.8(0.75) = 0.6$$

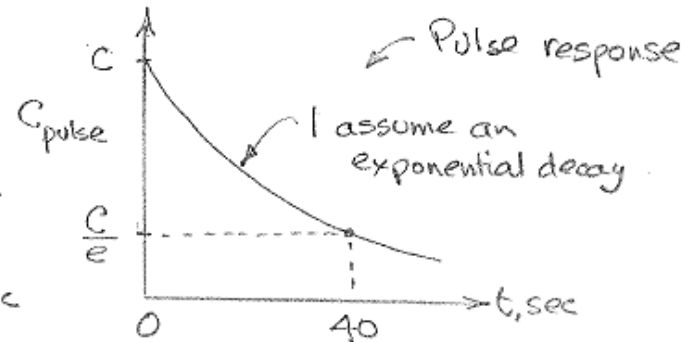
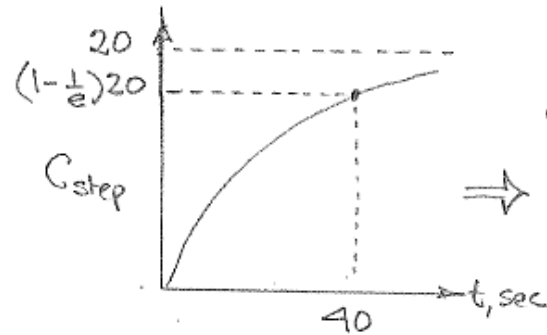
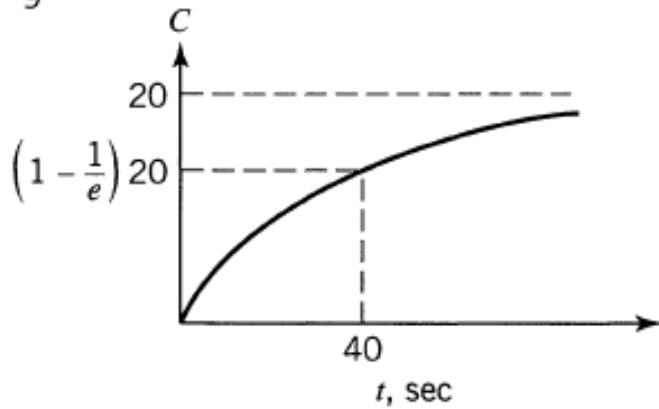
$$V_{p2} = U_2(2) = 0.2(2) = 0.4$$

note: no dead space

So the flow model is





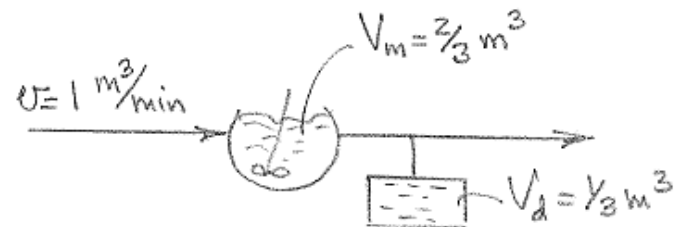


For mixed flow alone this should be 60sec. However, this curve comes out early, meaning dead spaces are present. This tracer curve shows that  $\bar{t} = 40$  sec, thus

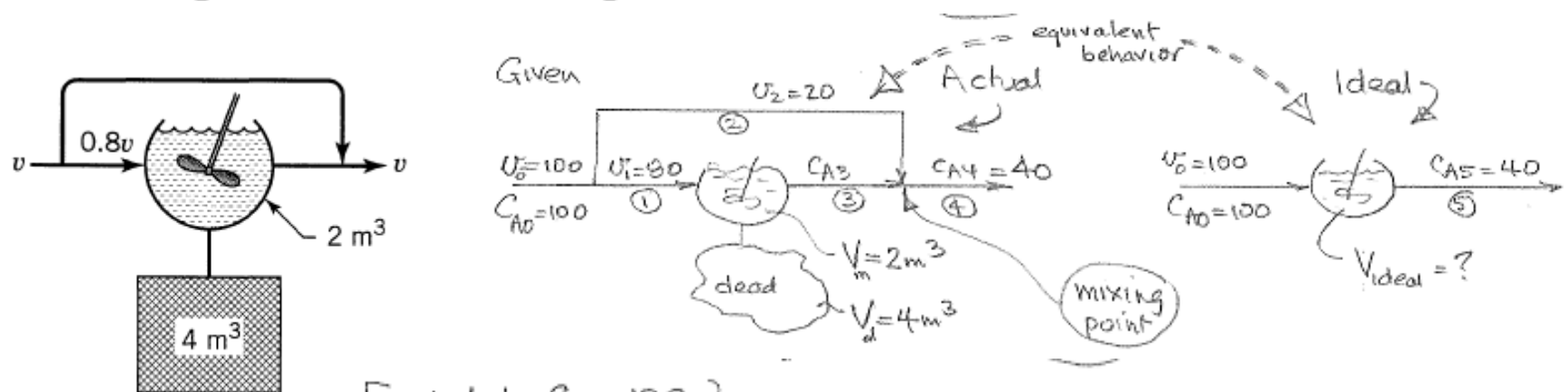
$$V_m = \frac{2}{3} \text{ m}^3$$

$$V_d = \frac{1}{3} \text{ m}^3$$

and our flow model is



**12.11.** The second order aqueous reaction  $A + B \rightarrow R + S$  is run in a large tank reactor ( $V = 6 \text{ m}^3$ ) and for an equimolar feed stream ( $C_{A0} = C_{B0}$ ) conversion of reactants is 60%. Unfortunately, agitation in our reactor is rather inadequate and tracer tests of the flow within the reactor give the flow model sketched in Fig. P12.11. What size of mixed flow reactor will equal the performance of our present unit?



First let  $C_{A0} = 100$   
 $v_0 = 100$  } It is not necessary to do this, but this assumption makes the calculations simpler.

Now take a material balance about the mixing point

$$v_2 C_{A2} + v_3 C_{A3} = v_4 C_{A4}$$

$$\text{or } 20(100) + 80 C_{A3} = 100(40)$$

$$\text{or } C_{A3} = \frac{100(40) + 20(100)}{80} = 75$$

Next evaluate the rate constant  $k$  from the actual  $2\text{m}^3$  MFR.  
For a 2<sup>nd</sup> order reaction



we have

$$\tau = \frac{V}{v} = \frac{C_{A0} - C_{A3}}{k C_{A3}^2}$$

or

$$k = \frac{C_{A0} - C_{A3}}{C_{A3}^2} \cdot \frac{v}{V} = \frac{100 - 75}{(75)^2} \cdot \frac{80}{2} = 14.222$$

Finally, for the ideal reactor

$$\frac{V_{\text{ideal}}}{v} = \frac{C_{A0} - C_{A5}}{k C_{A5}^2}$$

or

$$V_{\text{ideal}} = \frac{C_{A0} - C_{A5}}{k C_{A5}^2} \cdot v = \frac{100 - 40}{14.22 (40)^2} \cdot 100 = 0.2637 \text{m}^3$$

This is so much smaller than  $6\text{m}^3$