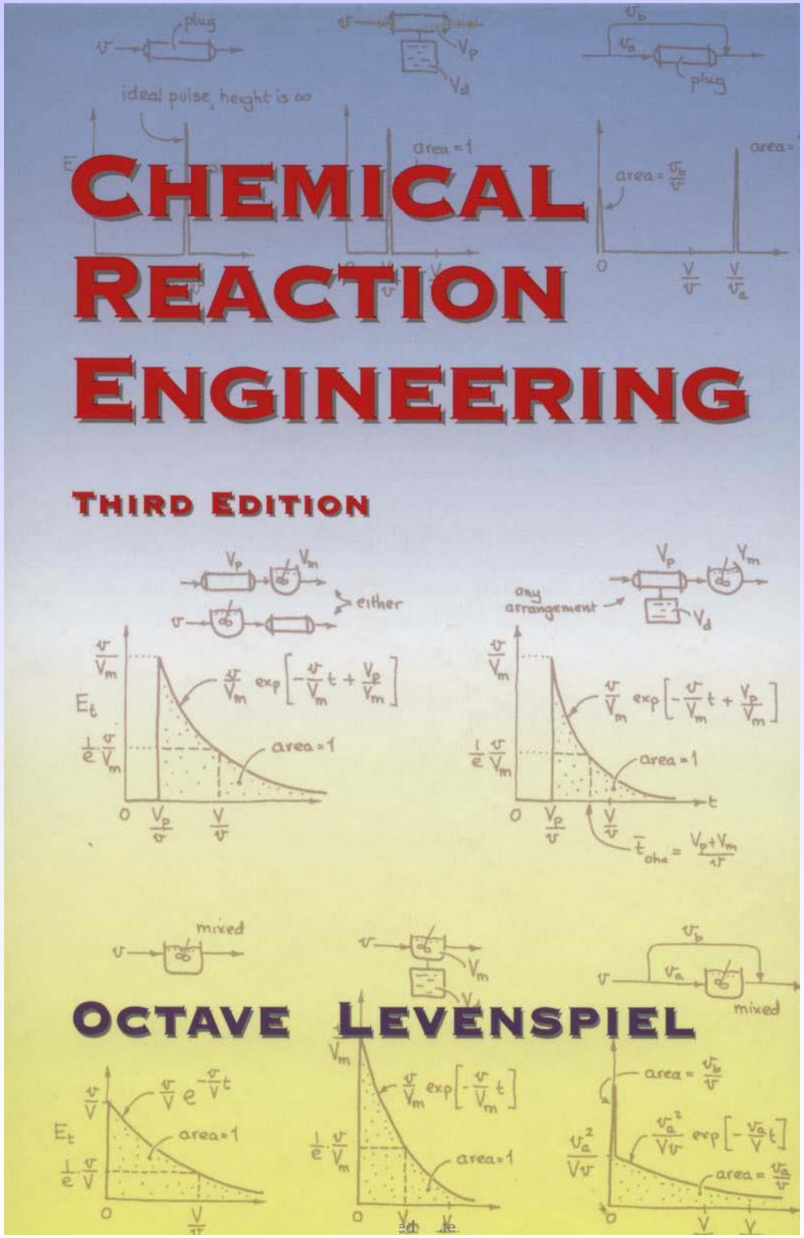
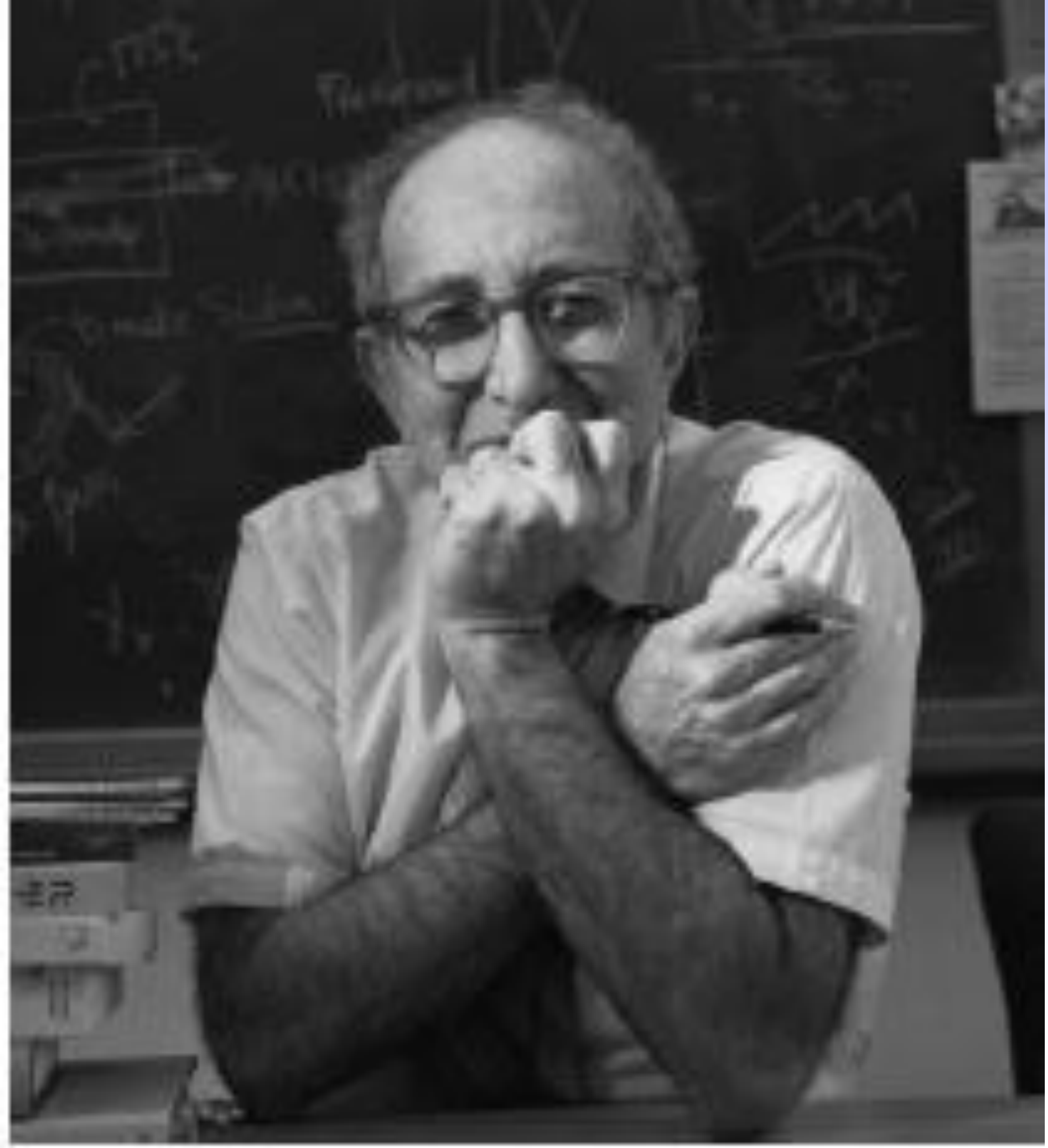


CHEMICAL REACTION ENGINEERING

THIRD EDITION

OCTAVE LEVENSPIEL



Education:

Ph.D. Chemical Engineering, Oregon State 1952
*M.S.*Chemical Engineering, Oregon State University, 1949
*B.S.*Chemistry, UC Berkeley, 1947

Interests and Research:

Octave Levenspiel served as a faculty member for 25 years until he retired in 1991. He authored 5 books and many papers and proceedings, two of which have been listed as "Citation Classics." He was awarded AIChE's 1977 W.K. Lewis Award, the 1979 R.H. Wilhelm Award, and the 2003 Founders Award and Gold Medal, the highest honor given by the society. In 2000 he was inducted into the National Academy of Engineering. He also received two honorary doctorates, one from France. He is known as the founder of Chemical Reaction Engineering.

Chapter 11

Basics of Non-Ideal Flow

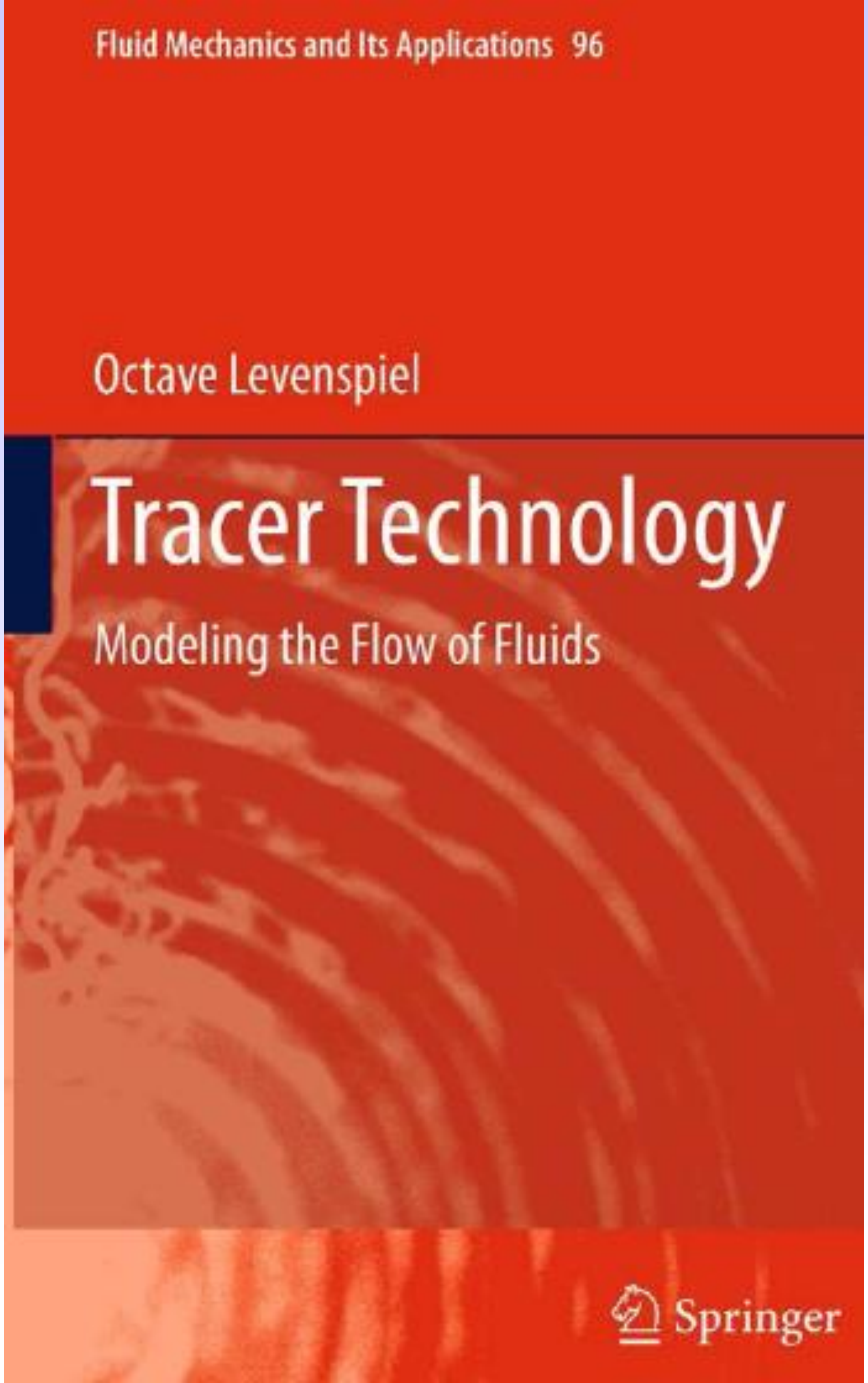
So far we have treated two flow patterns, plug flow and mixed flow. Most cases we try to design equipment to approach one or the other. But real equipment always deviates from these ideals.

In this chapter, we deals with:

RTD

state of aggregation

earliness and lateness of mixing



Fluid Mechanics and Its Applications 96

Octave Levenspiel

Tracer Technology

Modeling the Flow of Fluids

Springer

The Residence Time Distribution, RTD

- To simplify, we will only consider the steady-state flow, without reaction and without density change, of a single fluid through a vessel.

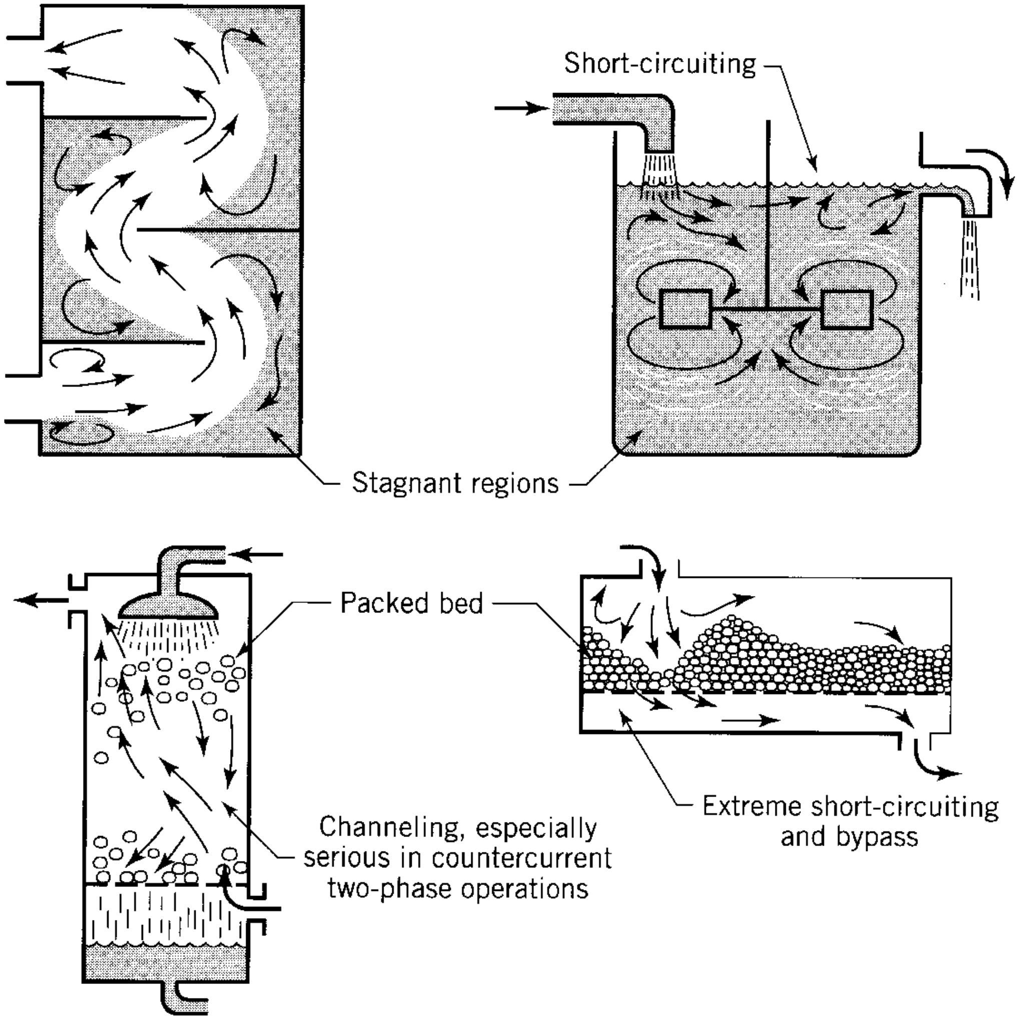


Figure 11.1 Nonideal flow patterns which may exist in process equipment.

- State of Aggregation of the Flowing Stream
- Microfluids and Macrofluids

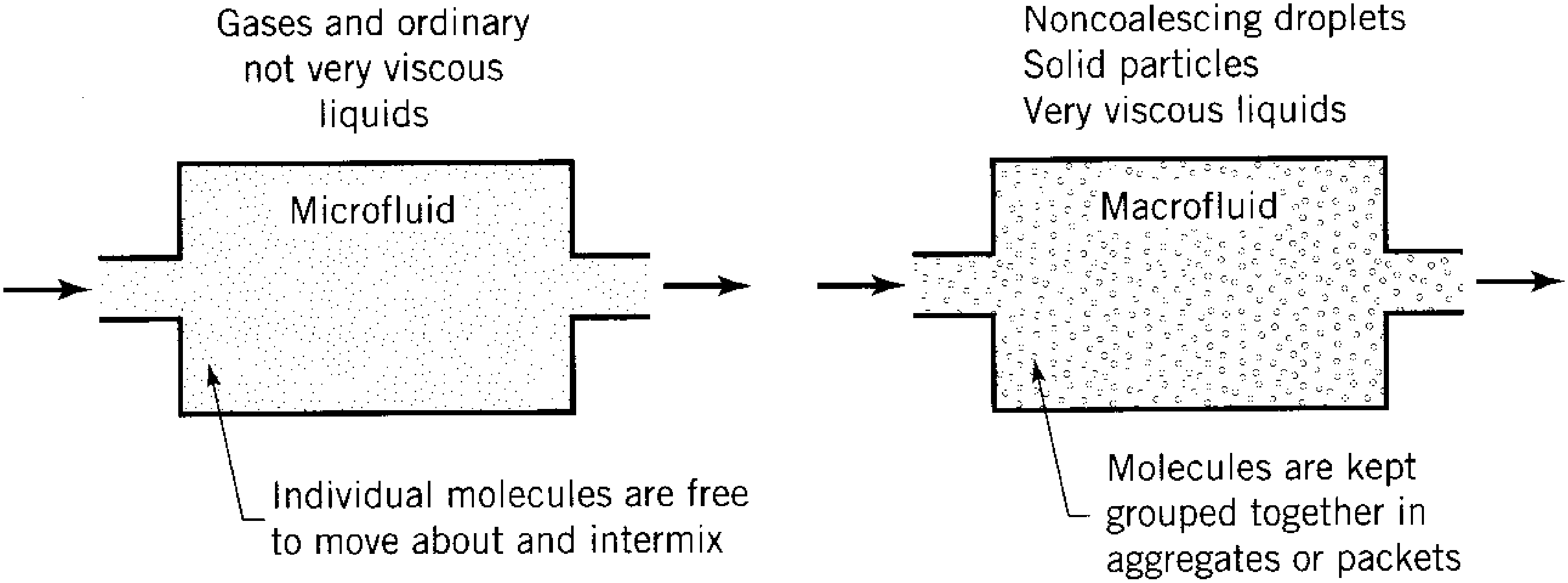


Figure 11.2 Two extremes of aggregation of fluid.

- Single-Phase Systems
- These lie somewhere between the extremes of macro- and microfluids.
- Two-Phase Systems
- A stream of solids always behaves as a macrofluid, but for gas reacting with liquid, either phase can be a macro- or microfluid depending on the contacting scheme being used.

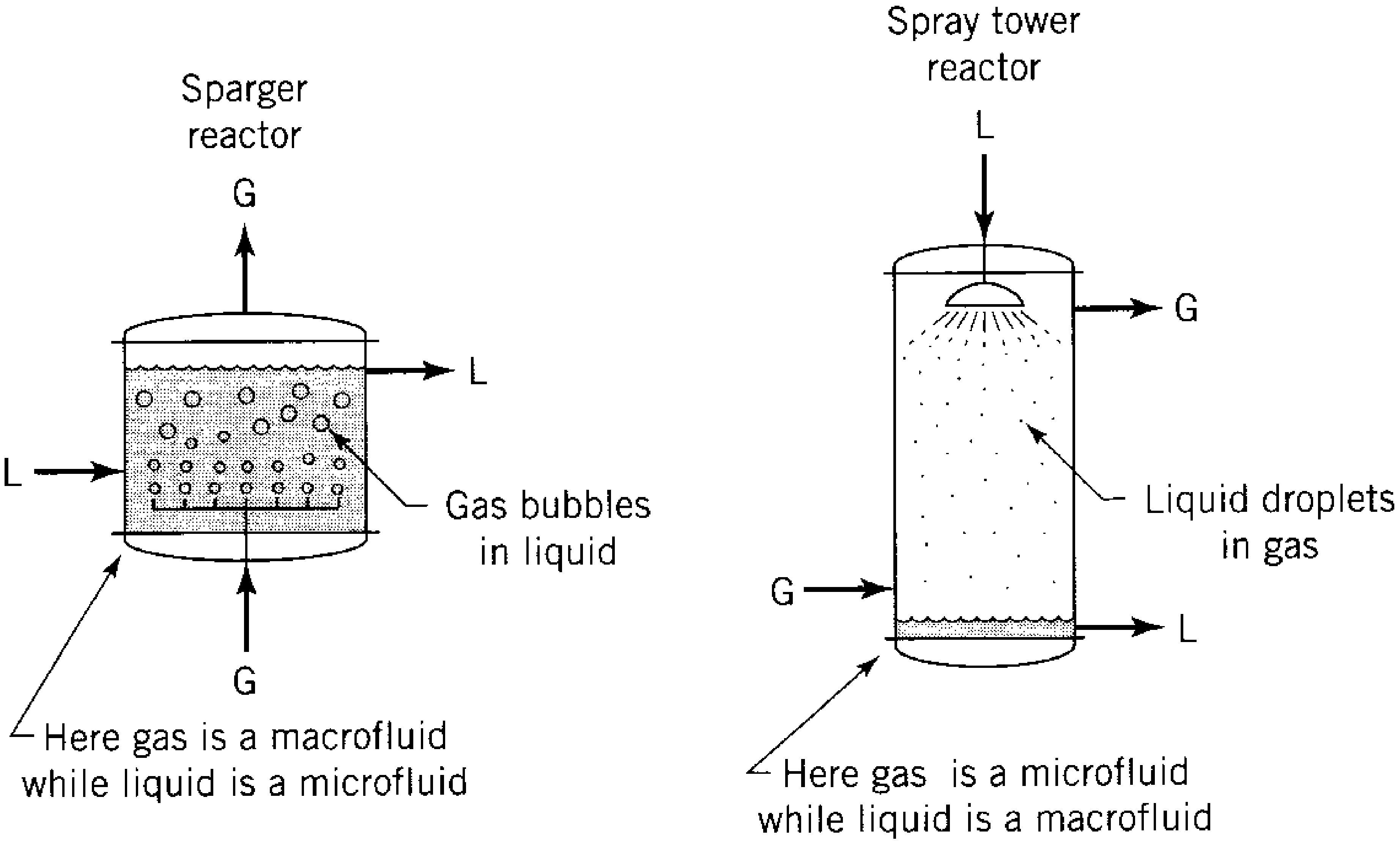


Figure 11.3 Examples of macro- and microfluid behavior.

- Earliness of Mixing
- the fluid elements of a single flowing stream can mix with each other either early or late in their flow through the vessel.

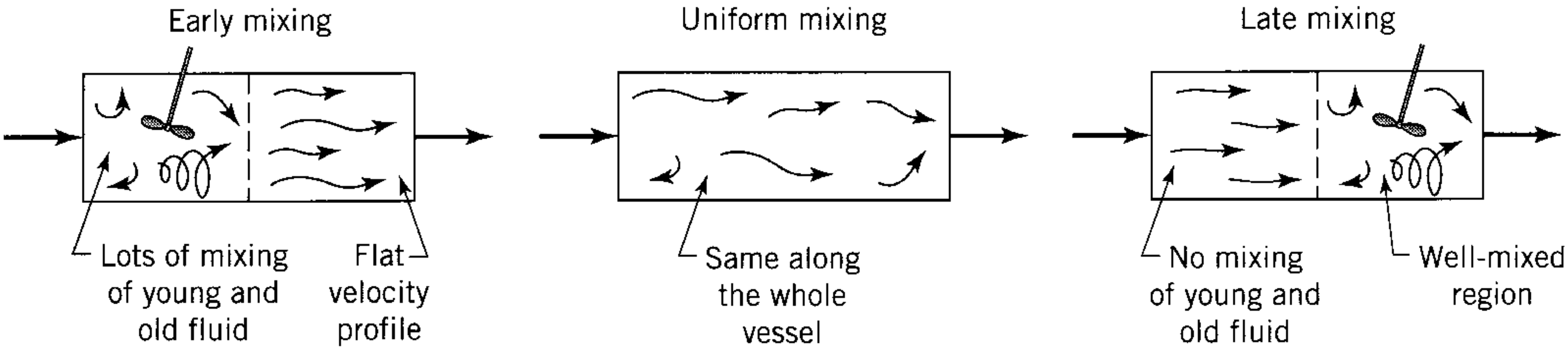
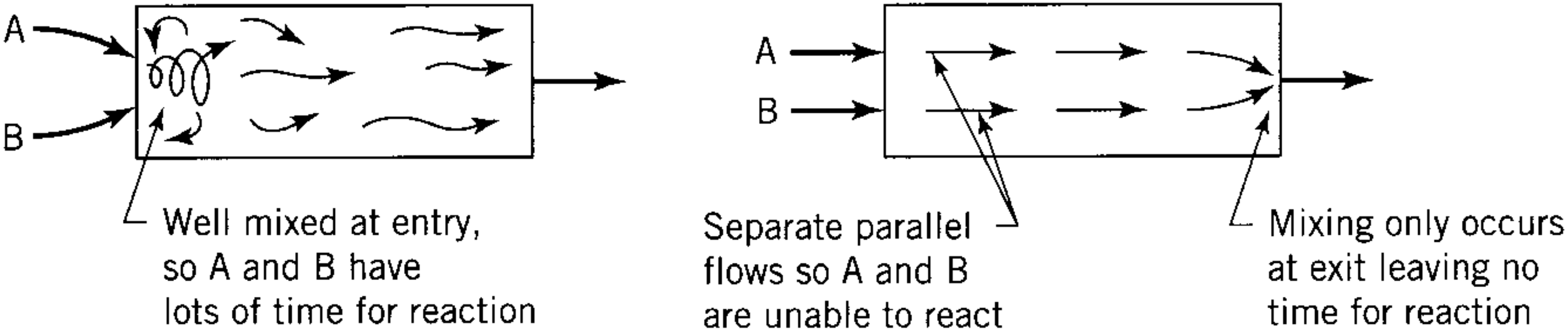


Figure 11.4 Examples of early and of late mixing of fluid.

- For a system with two entering reactant streams, earliness or lateness of mixing can be very important.



Well mixed at entry, so A and B have lots of time for reaction

Separate parallel flows so A and B are unable to react

Mixing only occurs at exit leaving no time for reaction

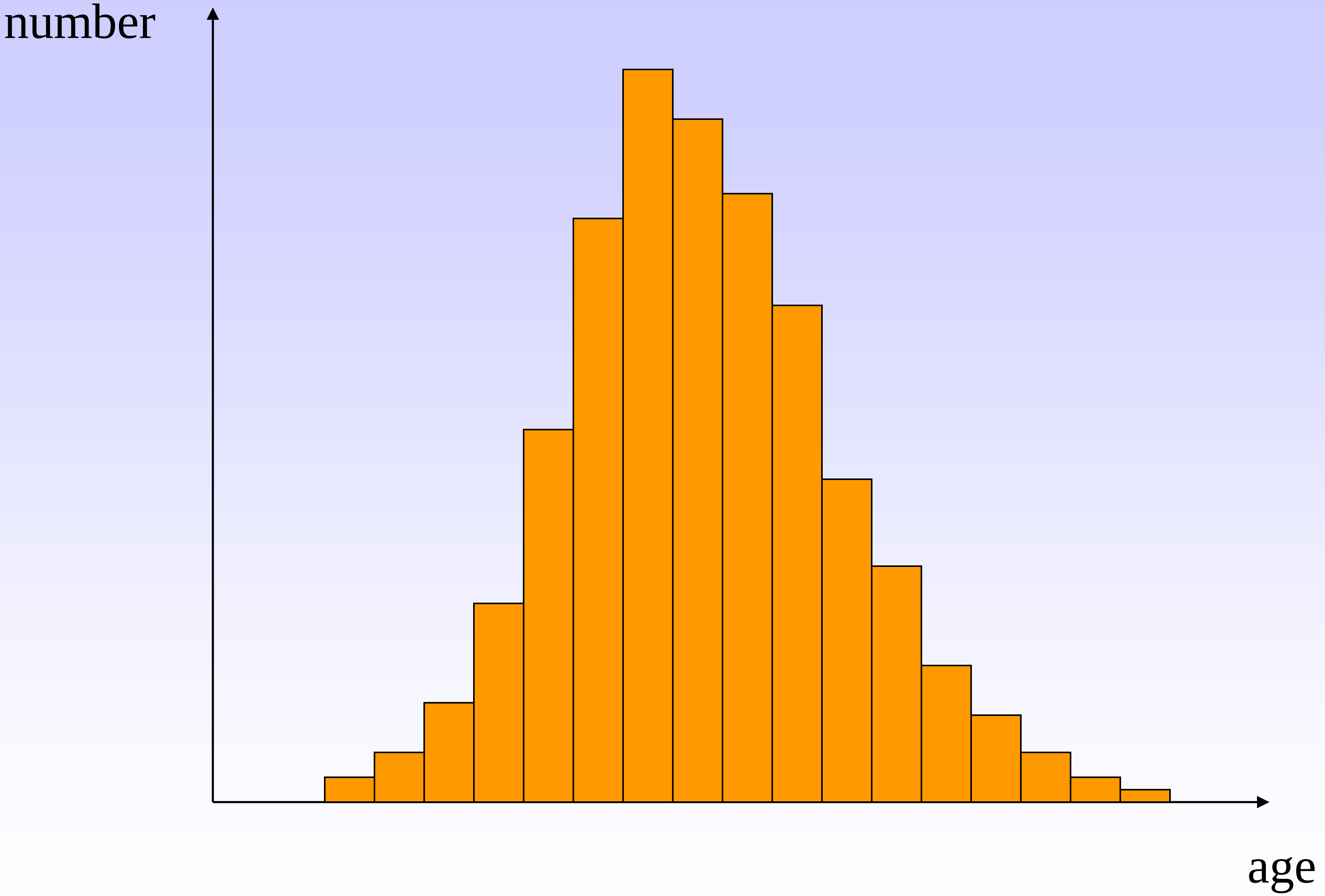
Figure 11.5 Early or late mixing affects reactor behavior.

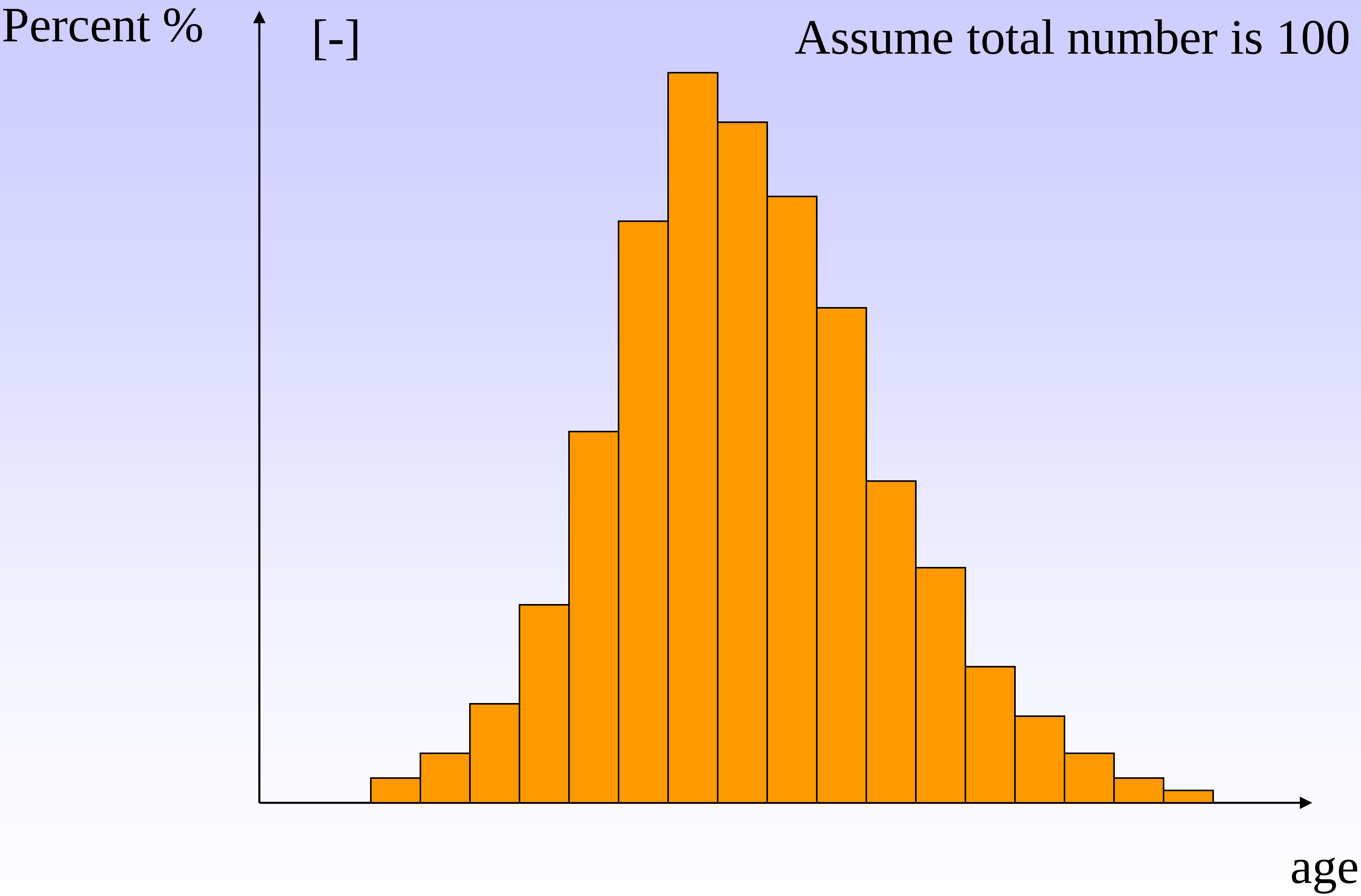
- Role of RTD, State of Aggregation, and Earliness of Mixing in Determining Reactor Behavior
- In some situations one of these three factors can be ignored, in others it can become crucial. Often, much depends on the time for reaction $\bar{t}_{rx}$, the time for mixing $\bar{t}_{mix}$, and the time for stay in the vessel $\bar{t}_{stay}$. In many cases $\bar{t}_{stay}$ has a meaning somewhat like $\bar{t}_{mix}$ but somewhat broader.

11.1 E, The Age Distribution of Fluid, the RTD

In this section, we do not consider any reaction

- It is evident that elements of fluid taking different routs through the reactor may take different lengths of time to pass through the vessel. The distribution of these times for the stream of fluid leaving the vessel is called the exit age distribution E, or the residence time distribution RTD of the fluid. E has the units of $time^{-1}$.

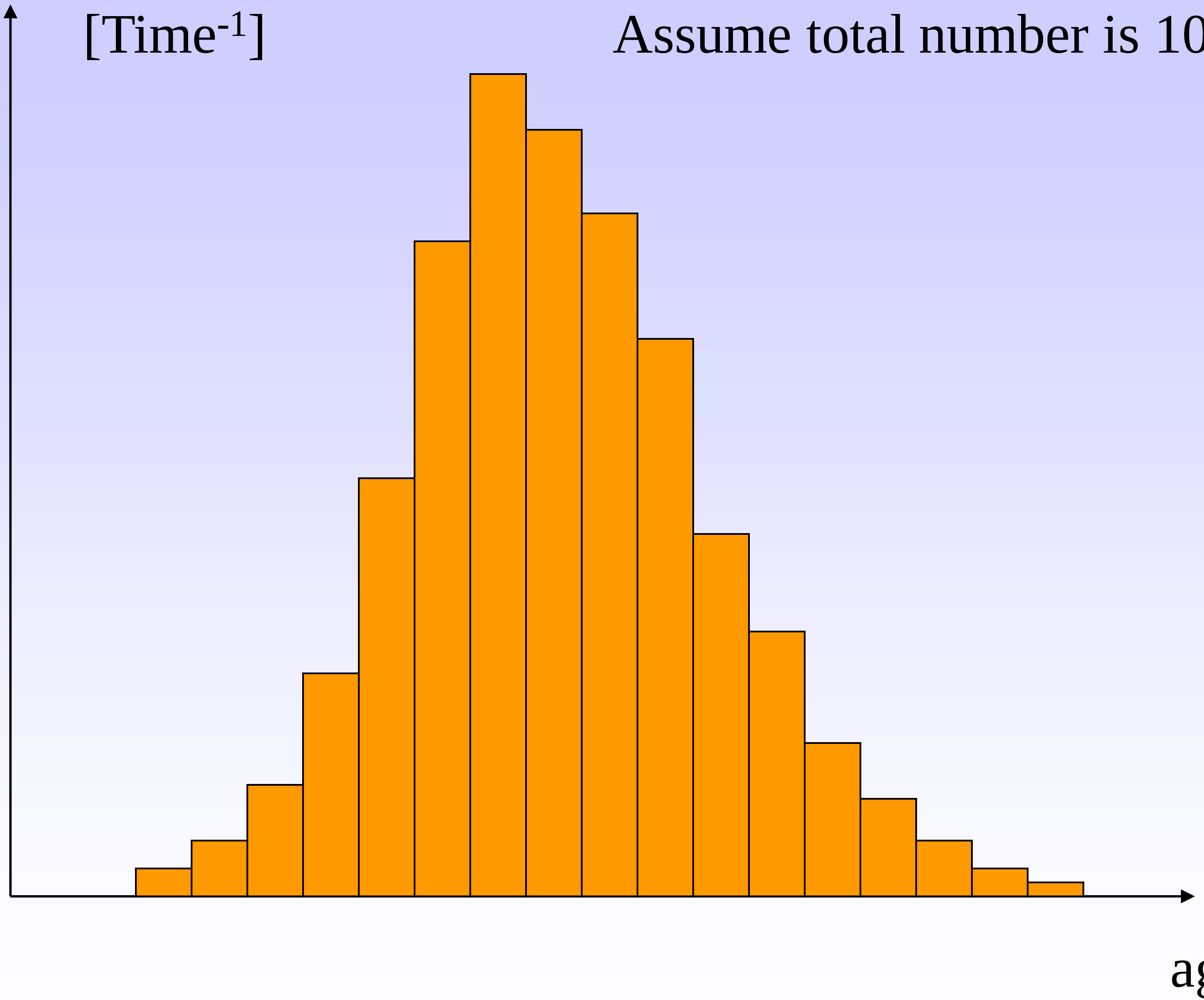

number
age

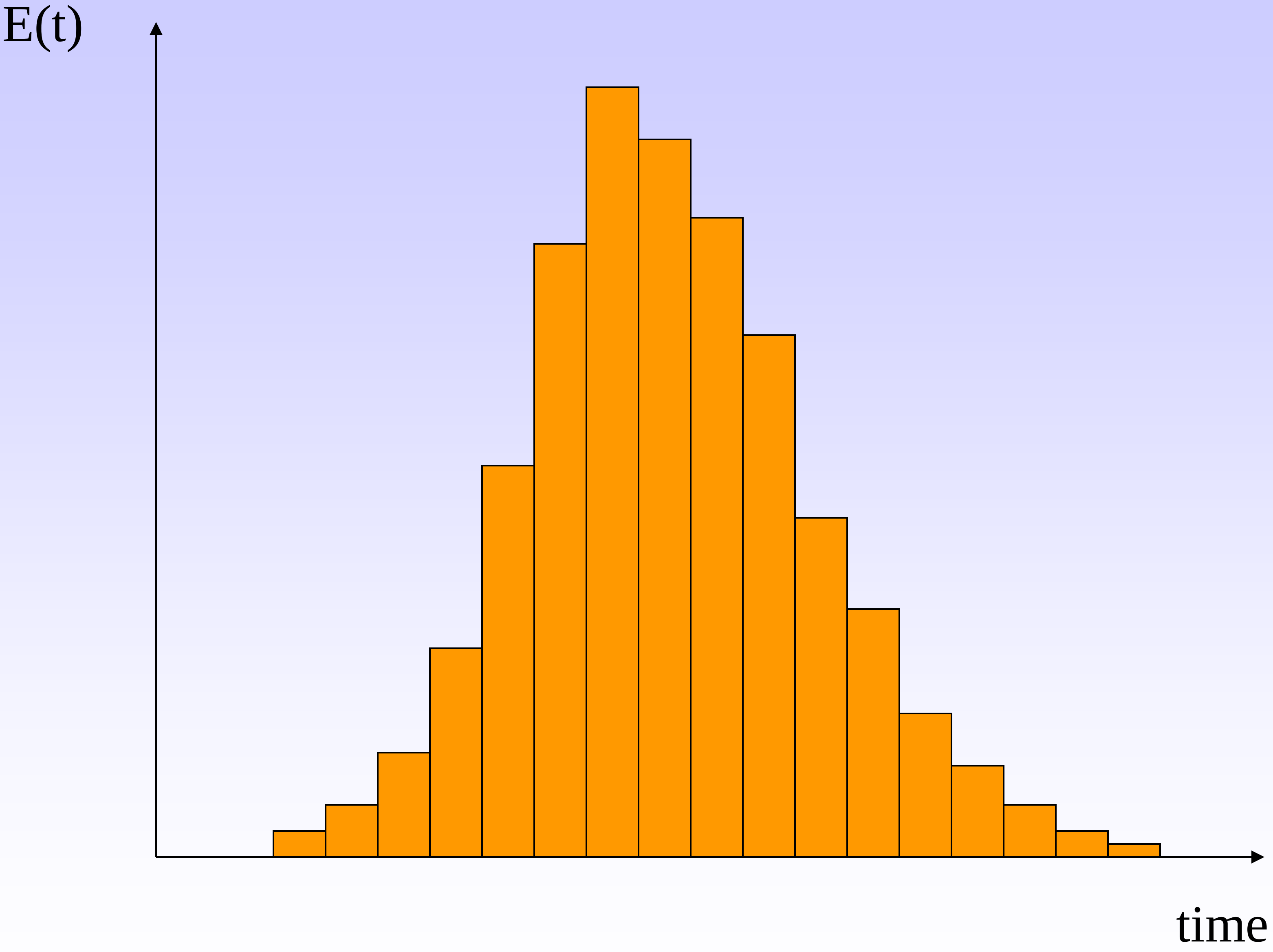


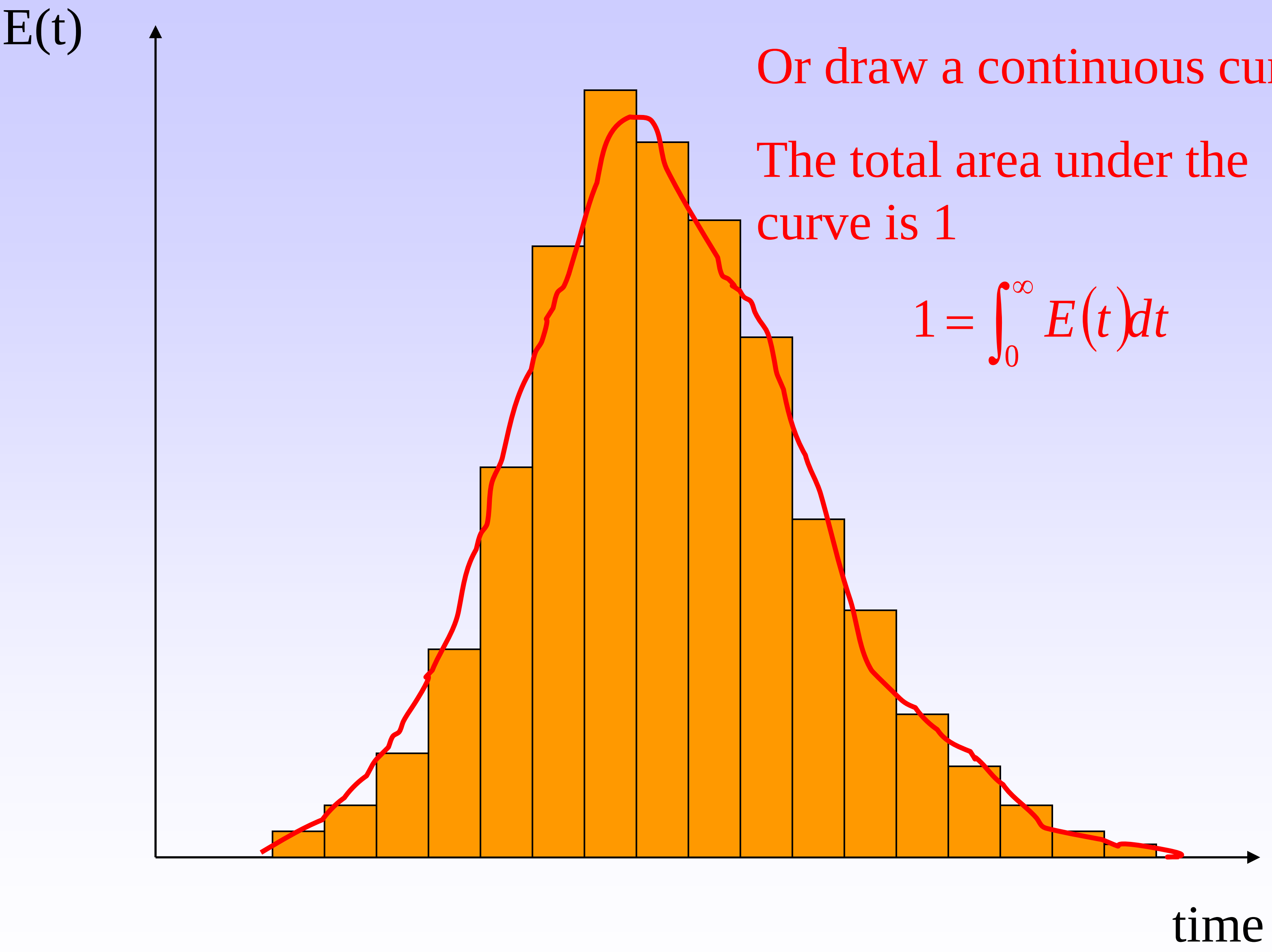
Assume total number is 100

$$\frac{\text{Percent \%}}{\Delta t}$$

Assume total number is 100



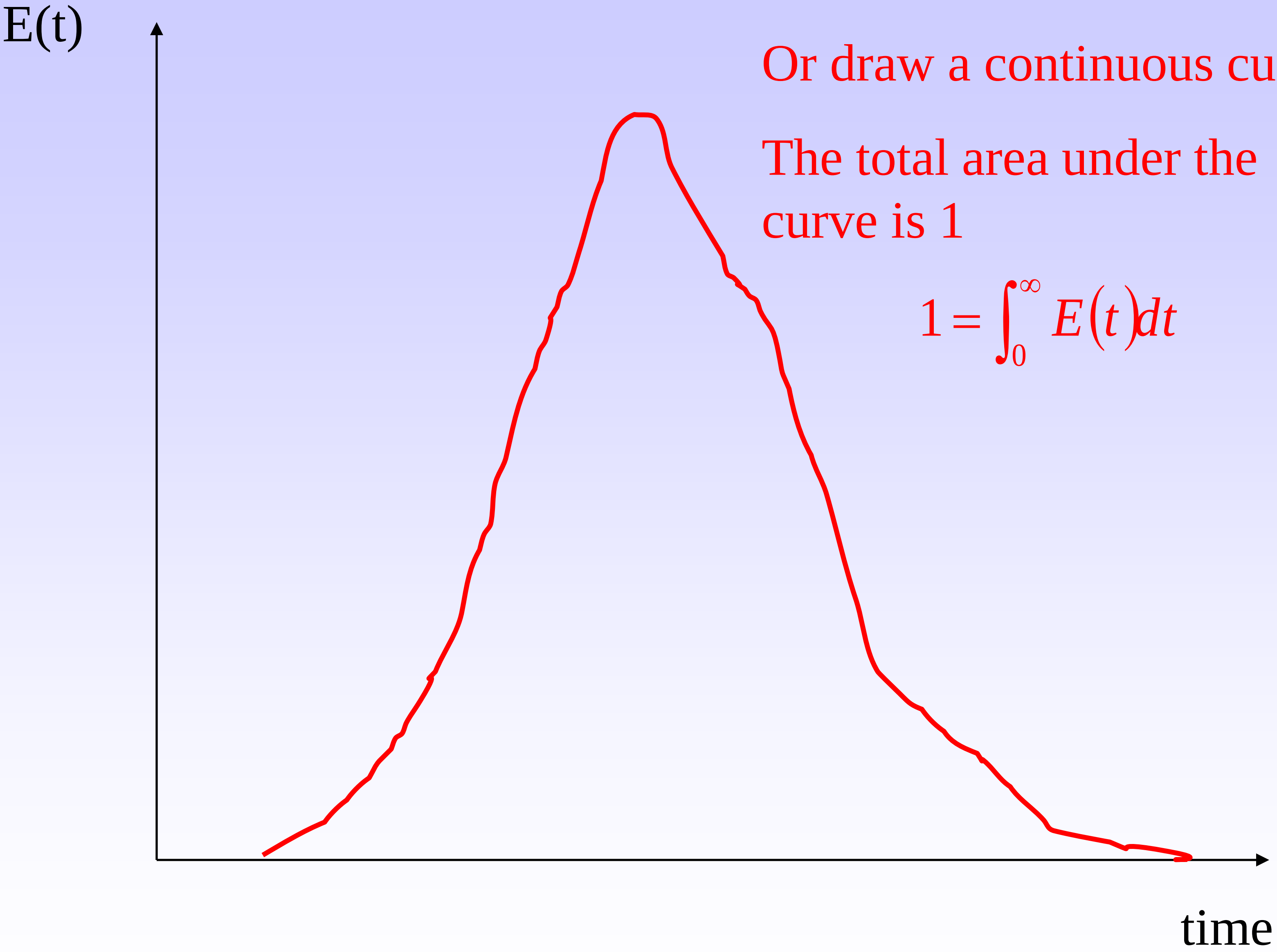

E(t)
time



Or draw a continuous curve

The total area under the curve is 1

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

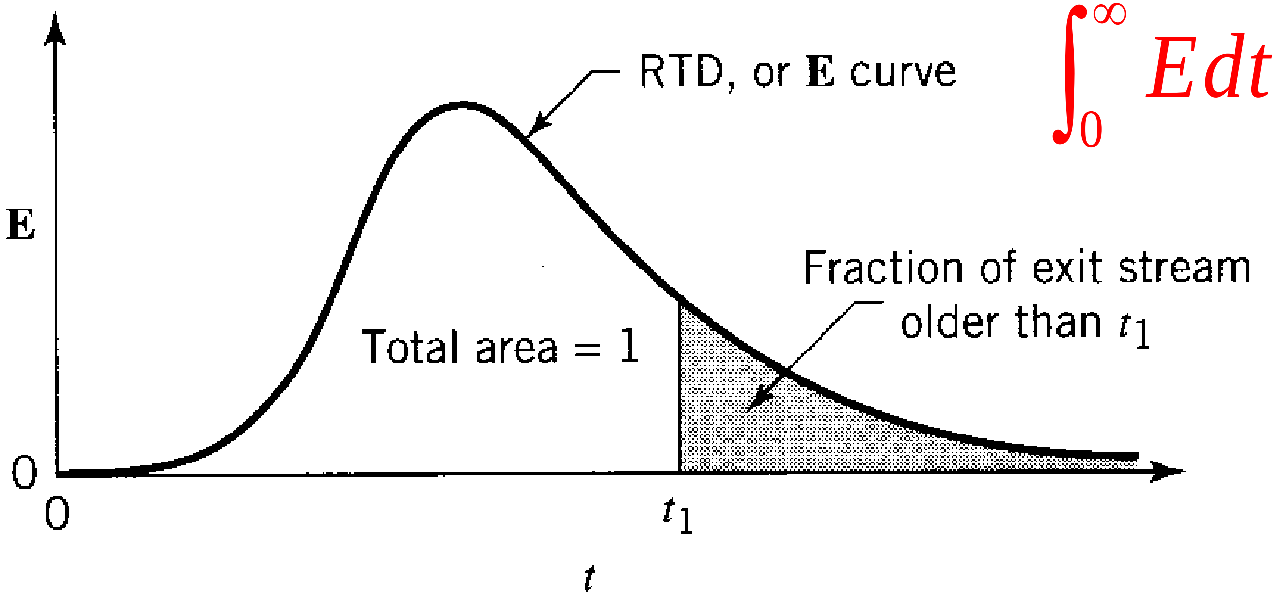


Or draw a continuous curve

The total area under the curve is 1

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

- We find it convenient to represent the RTD in such a way that the area under the curve is unity.



$$\int_0^{\infty} E\,dt = 1 \qquad [-]$$

Figure 11.6 The exit age distribution curve **E** for fluid flowing through a vessel; also called the residence time distribution, or RTD.

- With this representation the fraction of exit stream of age between t and $t+dt$ is

$$E\,dt \qquad [-]$$

The fraction younger than age t_1 is

$$\int_0^{t_1} E\,dt \qquad [-]$$

Whereas the fraction of material older than t_1 is

$$\int_{t_1}^{\infty} E\,dt = 1 - \int_0^{t_1} E\,dt \qquad [-]$$

- Experimental methods for finding E
- There are many methods to find the E curve. The simplest and most direct way is to use a physical or nonreactive tracer.
- Pulse and step experiments

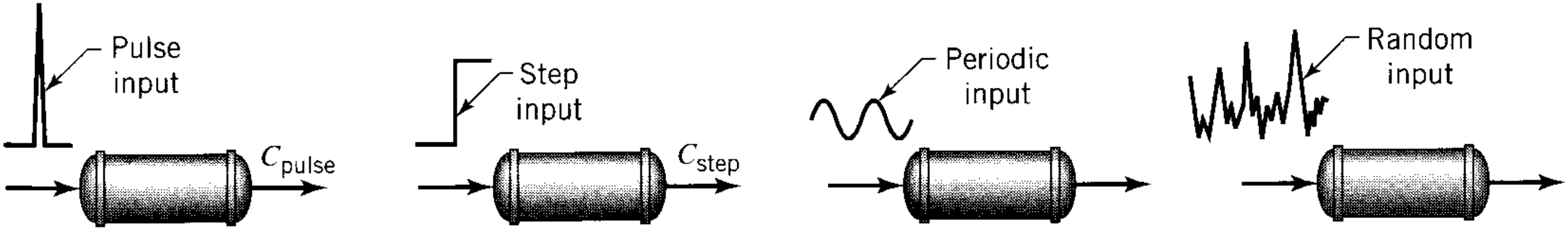


Figure 11.7 Various ways of studying the flow pattern in vessels.

The questions we ask of the tracer experiments are the following:

- Are there any dead, stagnant, or unused regions in the vessel?

- Is there any channeling or bypassing of fluid in the vessel?

- Is there any circulation of fluid within the vessel or out of and back into the vessel?

- Can we develop a reasonable flow model to represent the flow?

- The Pulse Experiment
- Let us find the E curve for a vessel of volume V m^3 through which flows v m^3/s of fluid. For instantaneously introduce M units of tracer (kg or mole) into the fluid entering the vessel, and record the concentration-time of tracer leaving the vessel. this is the C_{pulse} curve. From the material balance for the vessel we find

$$\begin{pmatrix}\text{Area under the} \\ \text{C}_{\text{pulse}}\text{ curve}\end{pmatrix}: \qquad A = \int_0^\infty C dt \cong \sum_i C_i \Delta t_i = \frac{M}{v} \qquad \left[\frac{kgs}{m^3}\right]$$

$$\begin{pmatrix}\text{Mean of the} \\ \text{C}_{\text{pulse}}\text{ curve}\end{pmatrix} \qquad \bar{t} = \frac{\int_0^\infty tCdt}{\int_0^\infty Cdt} \cong \frac{\sum_i tC_i \Delta t_i}{\sum_i C_i \Delta t_i} = \frac{V}{v} \qquad [s]$$

- To find E curve from C_{pulse} curve simply change the concentration scale such that the area under the curve is unity. Thus simply divide the concentration reading by M/*v.*

$$E = \frac{C_{pulse}}{M/v}$$

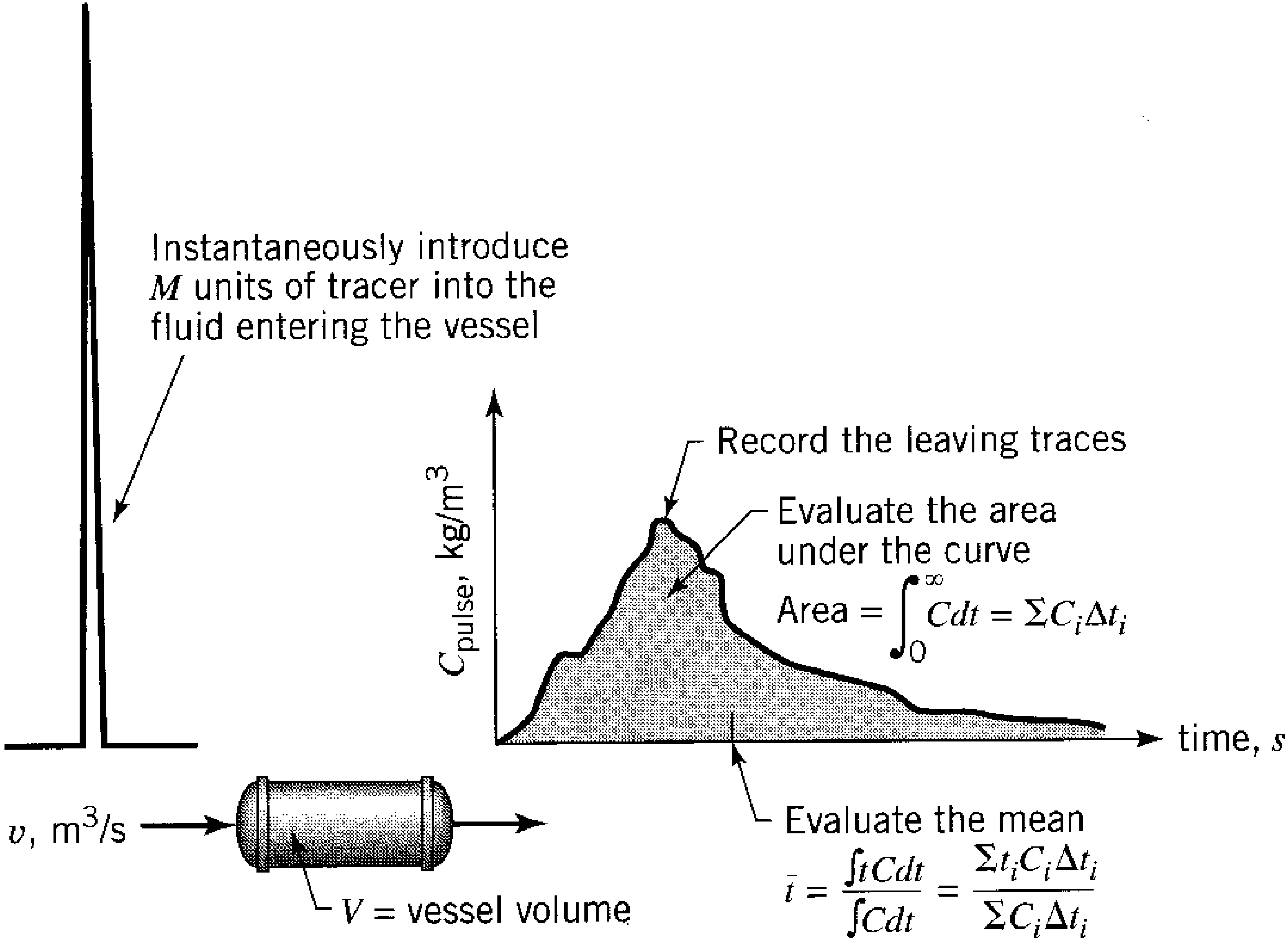


Figure 11.8 The useful information obtainable from the pulse trace experiment.

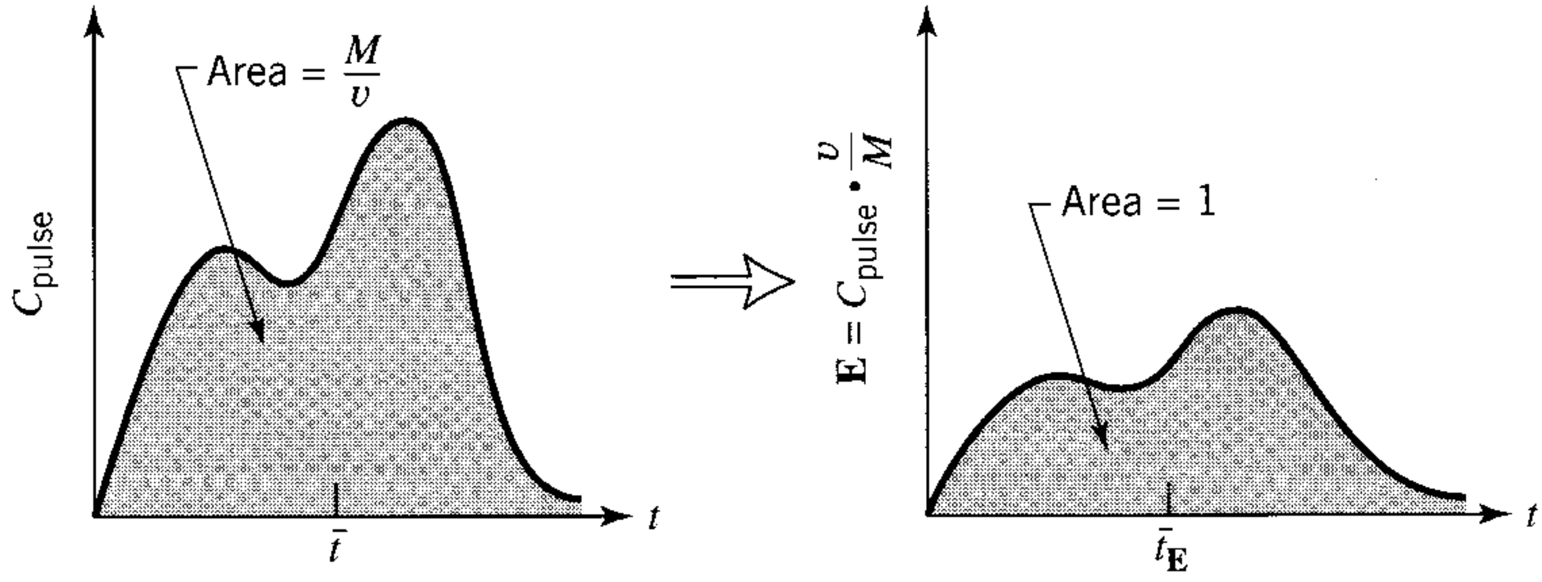


Figure 11.9 Transforming an experimental C_{pulse} curve into an **E** curve.

- We have another RTD function E_θ , Here time is measured in terms of mean residence time $\theta = t/\bar{t}$.

$$E_\theta = \bar{t}E = \frac{V}{v}\frac{C_{pulse}}{M/v} = \frac{V}{M}C_{pulse}$$

$$\left(\begin{array}{l} A = \frac{M}{v} \\ \bar{t} = \frac{V}{v} \end{array}\right)$$

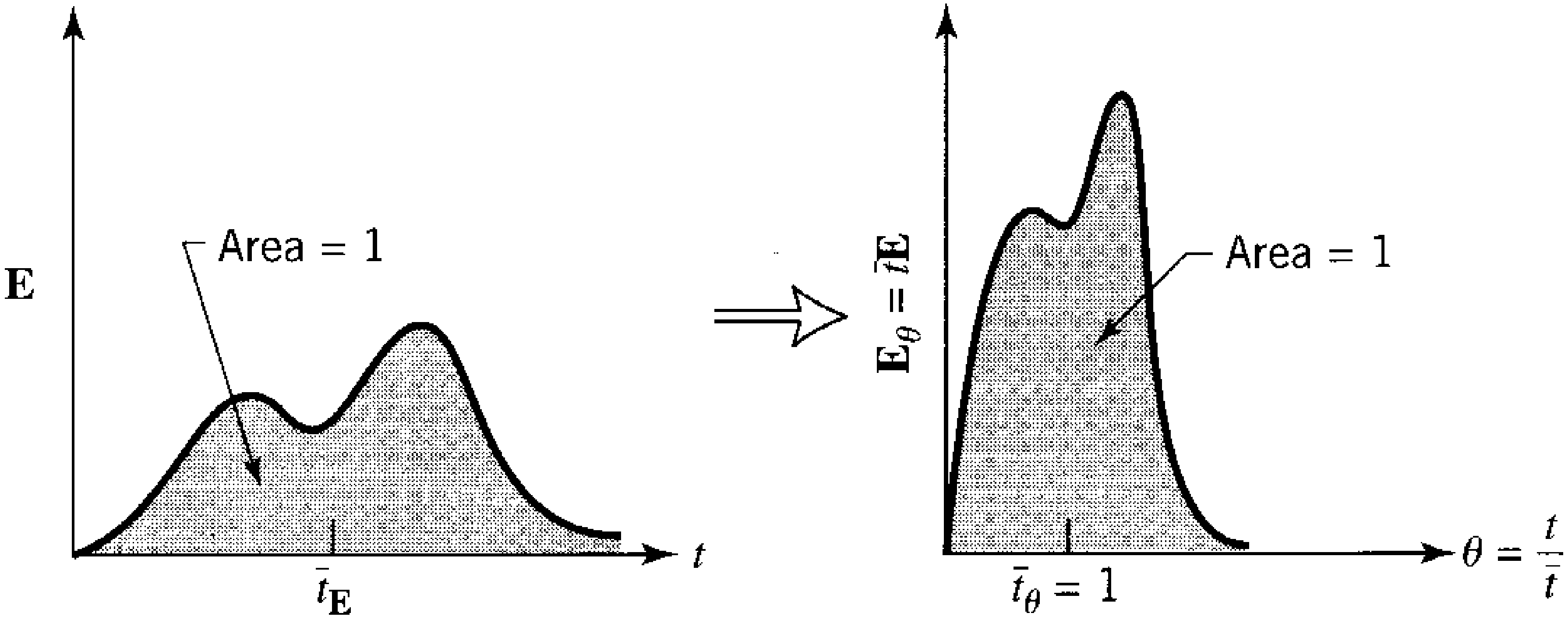


Figure 11.10 Transforming an **E** curve into an $\mathbf{E}_\theta$ curve.

- The Step Experiment
- Consider v m^3/s of fluid flowing through a vessel of volume V, Now at time $t=0$ switch from ordinary fluid to fluid with tracer of concentration $C_{\text{max}}=\left[\frac{\text{kg or mol}}{\text{m}^3}\right]$, and measure the outlet tracer concentration C_{step} vs. t.

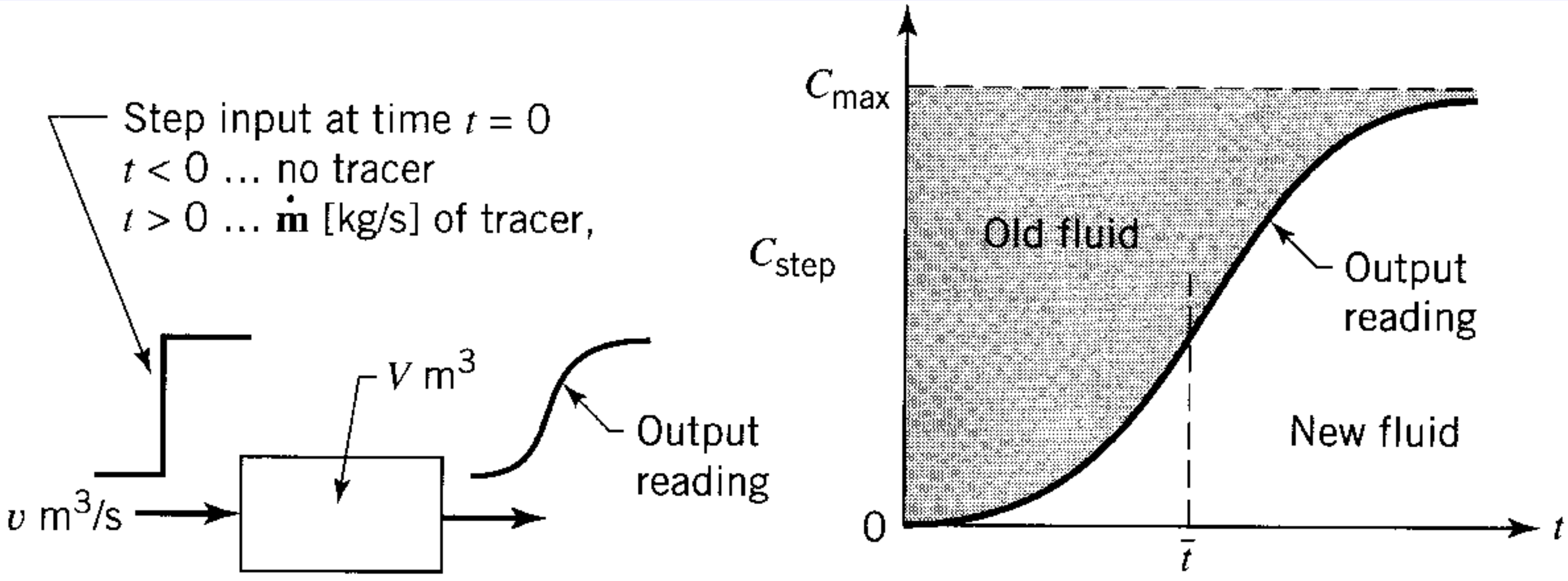


Figure 11.11 Information obtainable from a step tracer experiment.

- A material balance relates the different measured quantities of the output curve of a step input

$$C_{\max} = \frac{\dot{m}}{v} \qquad \left[\frac{kg}{m^3}\right] \quad \dot{m}\left[\mathrm{kg/s}\right] \text{is the flow rate of tracer in the entering fluid}$$

$$\begin{pmatrix}\text{shaded area}\\ \text{of fig. 11.11}\end{pmatrix} = C_{\max}\bar{t} = \frac{\dot{m}V}{v^2}\left[\frac{kg \cdot s}{m^3}\right]$$

$$\bar{t} = \frac{\int_0^{C_{\max}} t\,dC_{step}}{\int_0^{C_{\max}} dC_{step}} = \frac{1}{C_{\max}}\int_0^{C_{\max}} t\,dC_{step}$$

- Dimensionless form of the C_{step} is called the F curve.It is found by having the tracer concentration rise from zero to unity.

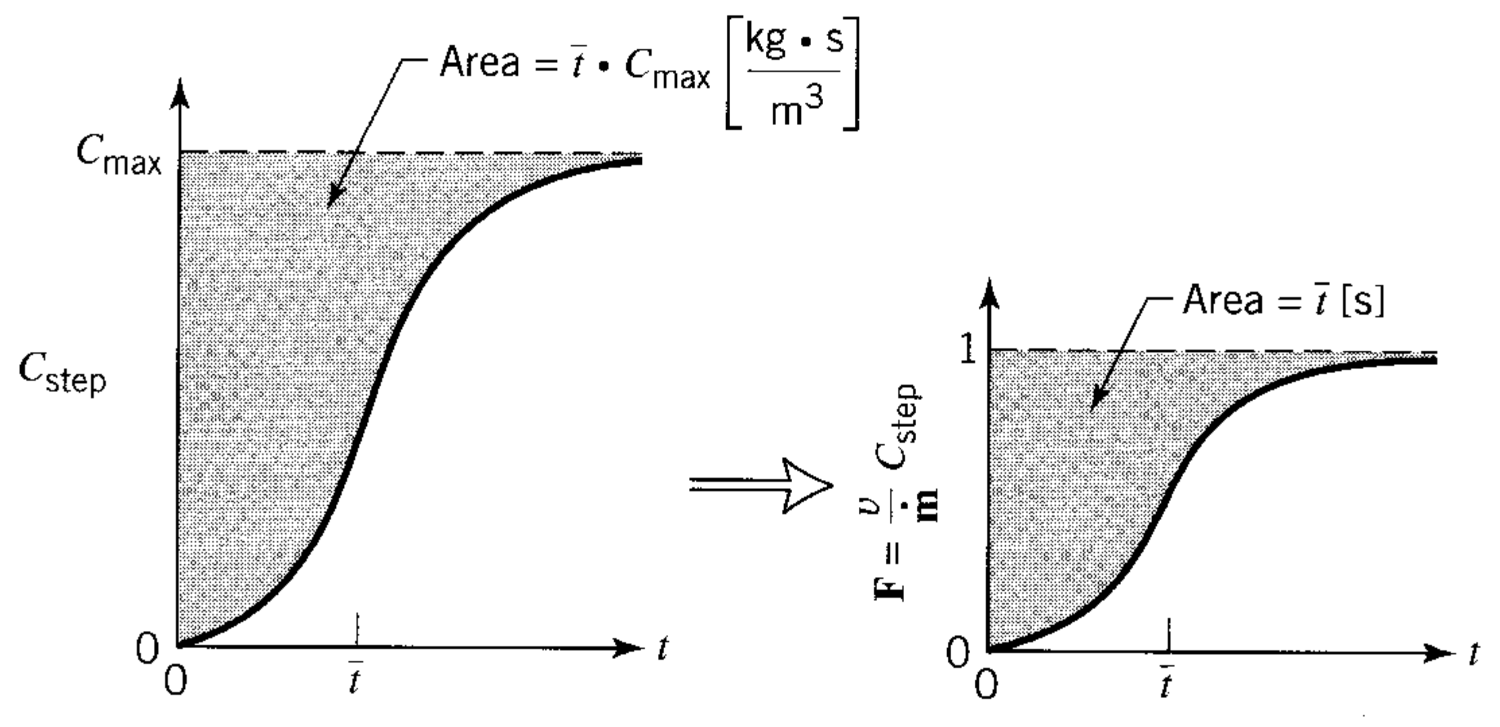
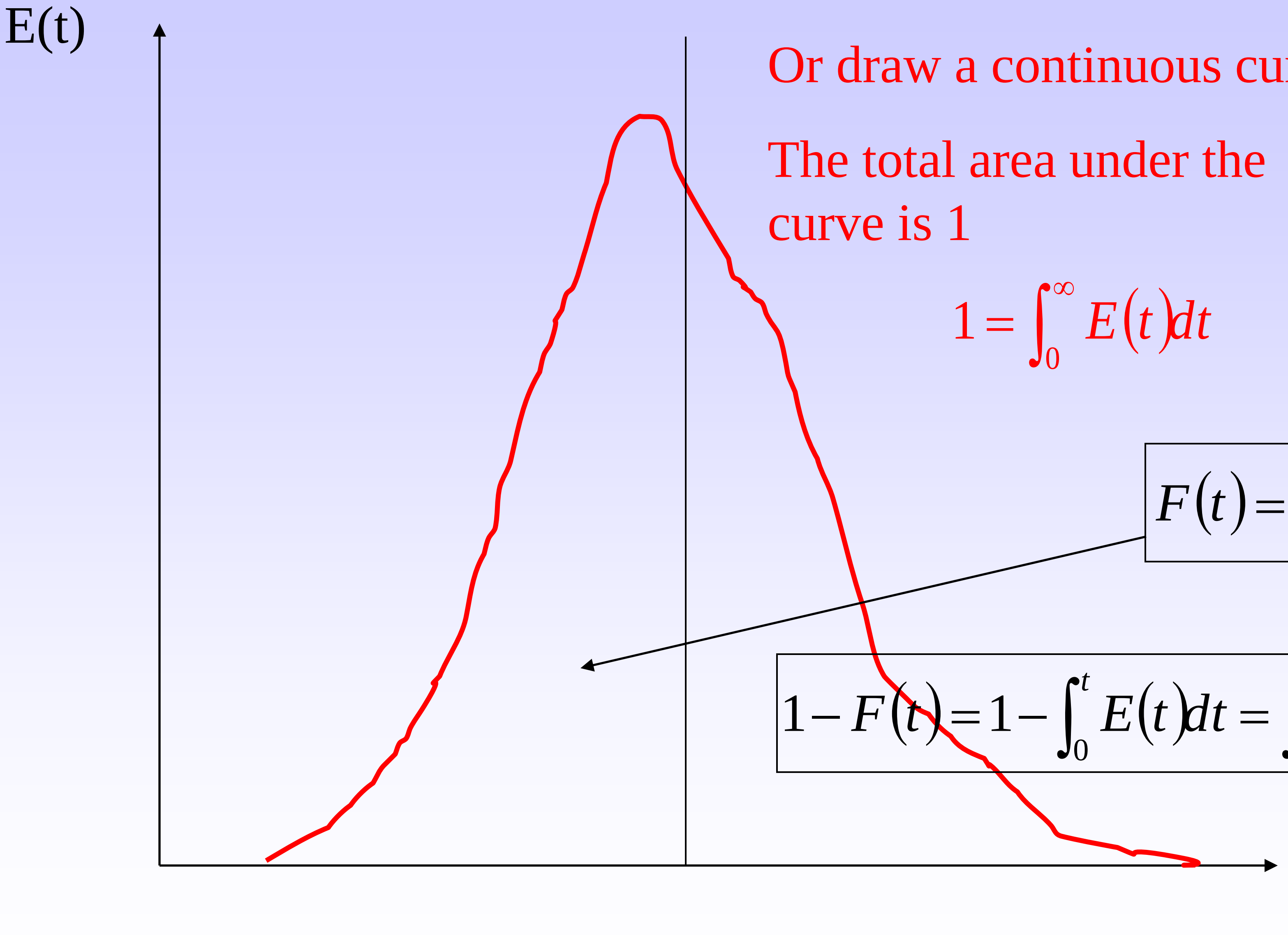


Figure 11.12 Transforming an experimental C_{step} curve to an **F** curve.

- Relationship between the F and the E curve
- To relate E with F, imagine a steady flow of white fluid. Then at time t=0 switch to red and record the rising concentration of red fluid in exit stream, the F curve. At any time t>0 red fluid and only red fluid in the exit stream is younger than age t. Thus we have

$$\underbrace{\begin{pmatrix}\text{fraction of red fluid}\\ \text{in the exit stream}\end{pmatrix}}_{F}=\underbrace{\begin{pmatrix}\text{fraction of exit stream}\\ \text{younger than age t}\end{pmatrix}}_{\int_0^t Edt}$$



Or draw a continuous curve

The total area under the curve is 1

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

$$\boxed{F(t) = \int_0^t E(t)\,dt}$$

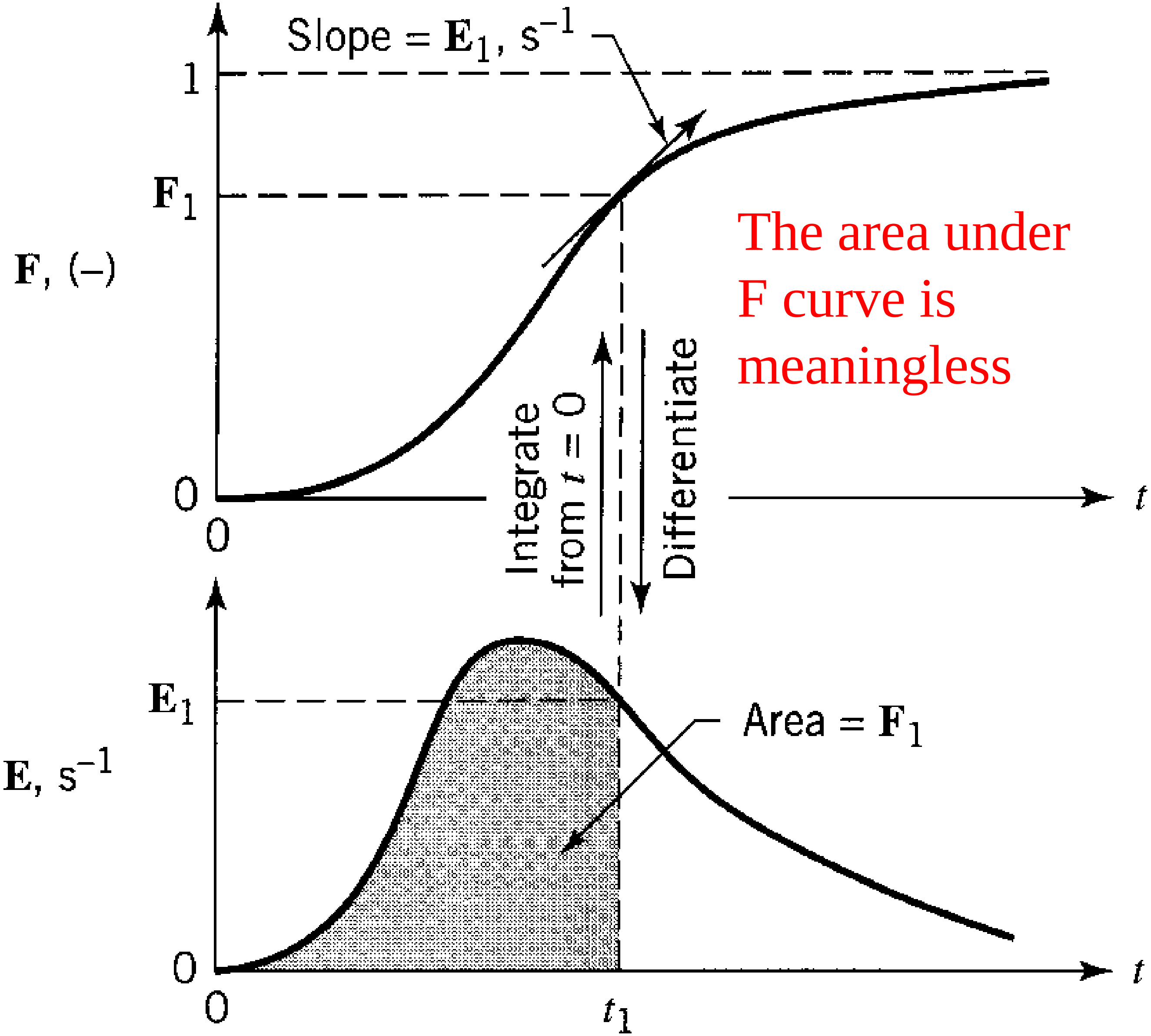
$$\boxed{1 - F(t) = 1 - \int_0^t E(t)\,dt = \int_t^\infty E(t)\,dt}$$

So we get

$$F = \int_0^t E\,dt$$

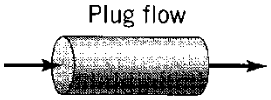
and

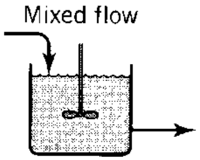
$$\frac{dF}{dt} = E$$

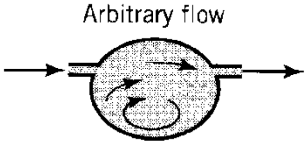


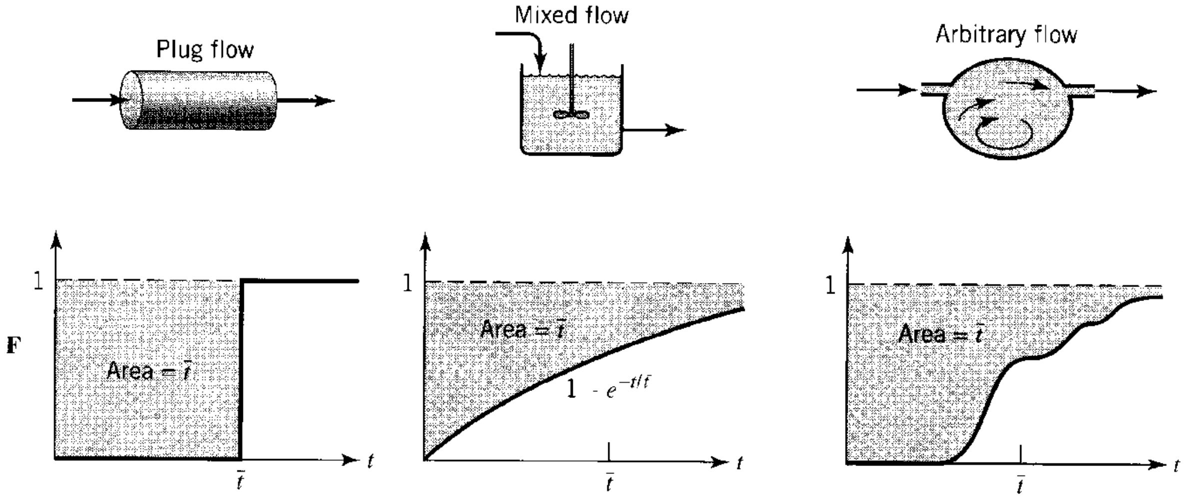
The area under F curve is meaningless

Figure 11.13 Relationship between the **E** and **F** curves.


Plug flow


Mixed flow


Arbitrary flow


Plug flow
Mixed flow
Arbitrary flow
1
F
Area = $\bar{t}$
$\bar{t}$
t
1
Area = $\bar{t}$
$1 - e^{-t/\bar{t}}$
$\bar{t}$
t
1
Area = $\bar{t}$
$\bar{t}$
t

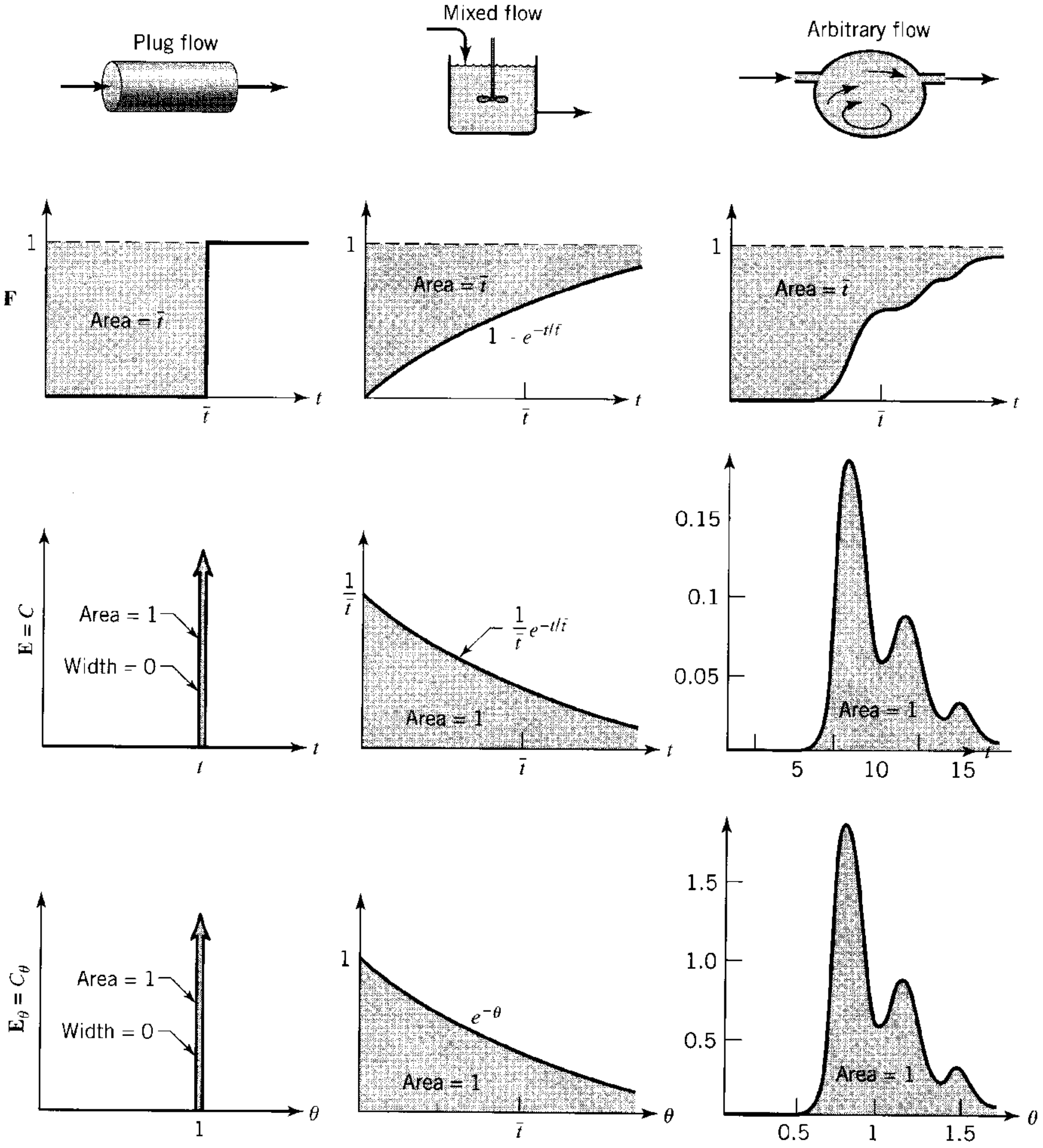


Figure 11.14 Properties of the **E** and **F** curves for various flows. Curves are drawn in terms of ordinary and dimensionless time units. Relationship between curves is given by Eqs. 7 and 8.

The Dirac Delta Function

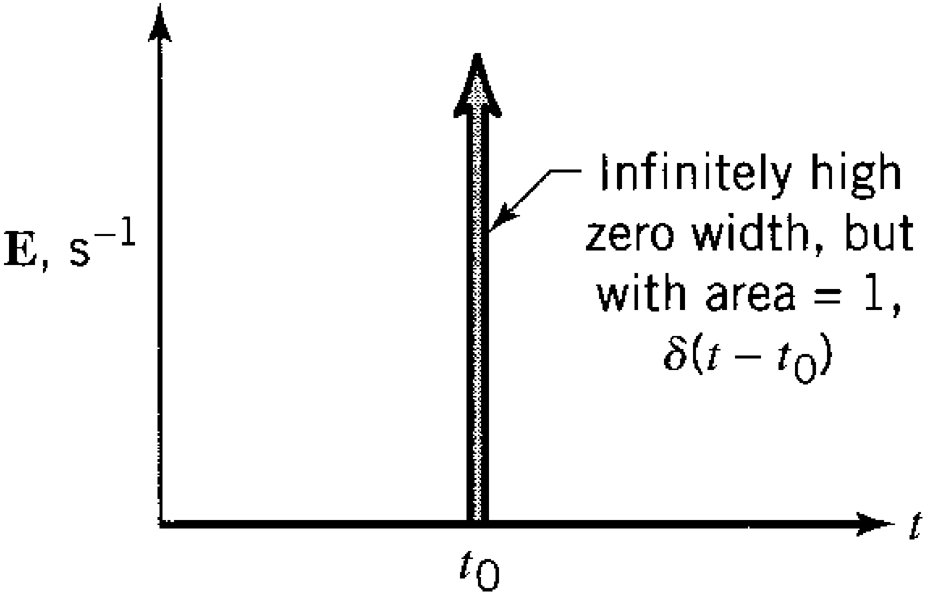


Figure 11.18 The **E** function for plug flow.

$$\delta\left(t-t_0\right)$$

$$\int_0^\infty \delta\left(t-t_0\right)dt=1$$

$$\int_0^\infty \delta\left(t-t_0\right)f(t)dt=f(t_0)$$

EXAMPLE 11.1 FINDING THE RTD BY EXPERIMENT

The concentration readings in Table E11.1 represent a continuous response to a pulse input into a closed vessel which is to be used as a chemical reactor. Calculate the mean residence time of fluid in the vessel t, and tabulate and plot the exit age distribution **E**.

Table E11.1

Time t, min	Tracer Output Concentration, C_{pulse} gm/liter fluid
0	0
5	3
10	5
15	5
20	4
25	2
30	1
35	0

SOLUTION

The mean residence time, from Eq. 4, is

$$\bar{t} = \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i} \xlongequal{\Delta t = \text{constant}} \frac{\sum t_i C_i}{\sum C_i}$$

$$= \frac{5 \times 3 + 10 \times 5 + 15 \times 5 + 20 \times 4 + 25 \times 2 + 30 \times 1}{3 + 5 + 5 + 4 + 2 + 1} = 15 \text{ min}$$

The area under the concentration-time curve,

$$\text{Area} = \sum C \, \Delta t = (3 + 5 + 5 + 4 + 2 + 1)5 = 100 \text{ gm} \cdot \text{min/liter}$$

gives the total amount of tracer introduced. To find **E**, the area under this curve must be unity; hence, the concentration readings must each be divided by the total area, giving

$$\mathbf{E} = \frac{C}{\text{area}}$$

Thus we have

t, min	0	5	10	15	20	25	30
$\mathbf{E} = \dfrac{C}{\text{area}}$, min^{-1}	0	0.03	0.05	0.05	0.04	0.02	0.01

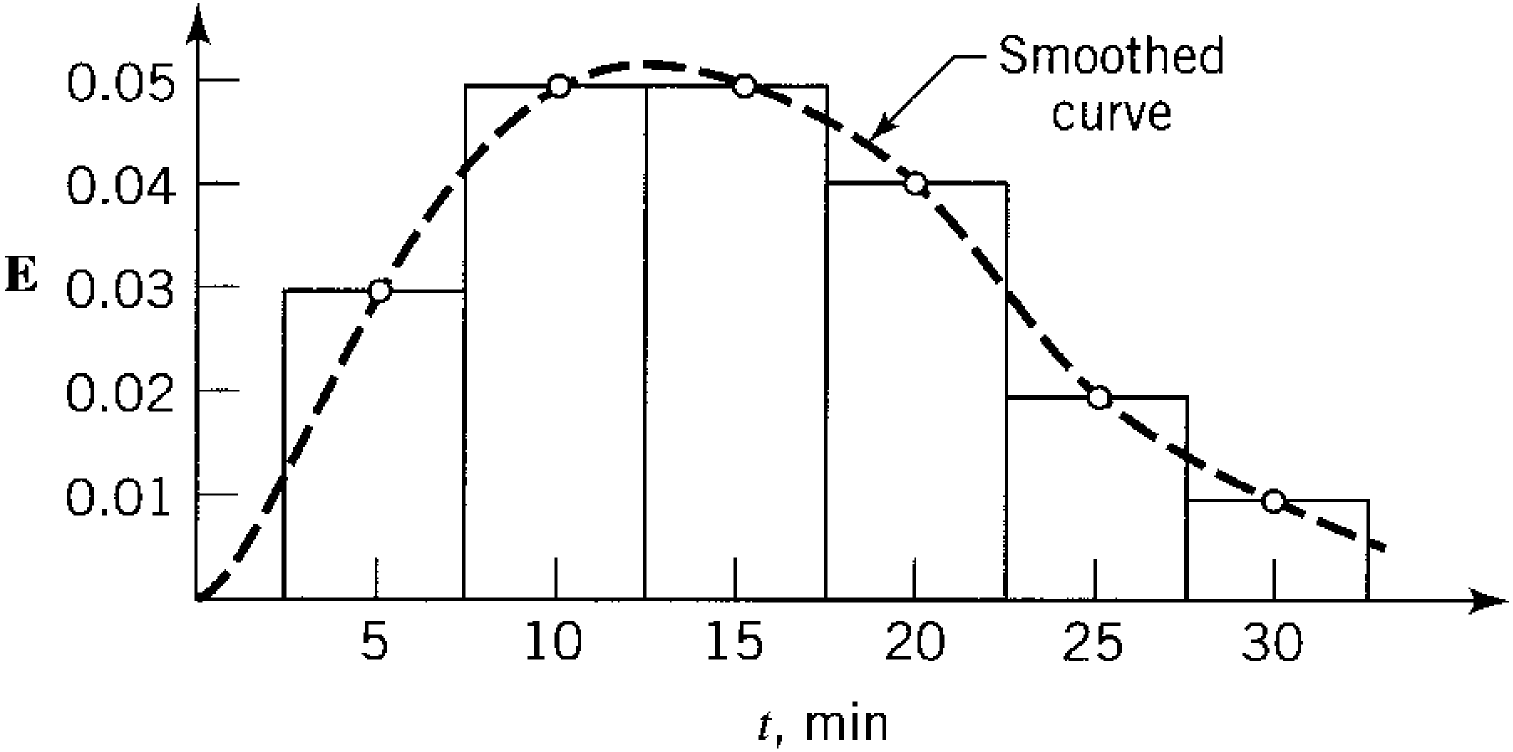


Figure E11.1

EXAMPLE 11.2 *FINDING THE E CURVE FOR LIQUID FLOWING THROUGH A VESSEL*

A large tank (860 liters) is used as a gas-liquid contactor. Gas bubbles up through the vessel and out the top, liquid flows in at one part and out the other at 5 liters/s. To get an idea of the flow pattern of liquid in this tank a pulse of tracer ($M = 150$ gm) is injected at the liquid inlet and measured at the outlet, as shown in Fig. E11.2*a*.

(a) Is this a properly done experiment?
(b) If so, find the liquid fraction in the vessel.
(c) Determine the **E** curve for the liquid.
(d) Qualitatively what do you think is happening in the vessel?

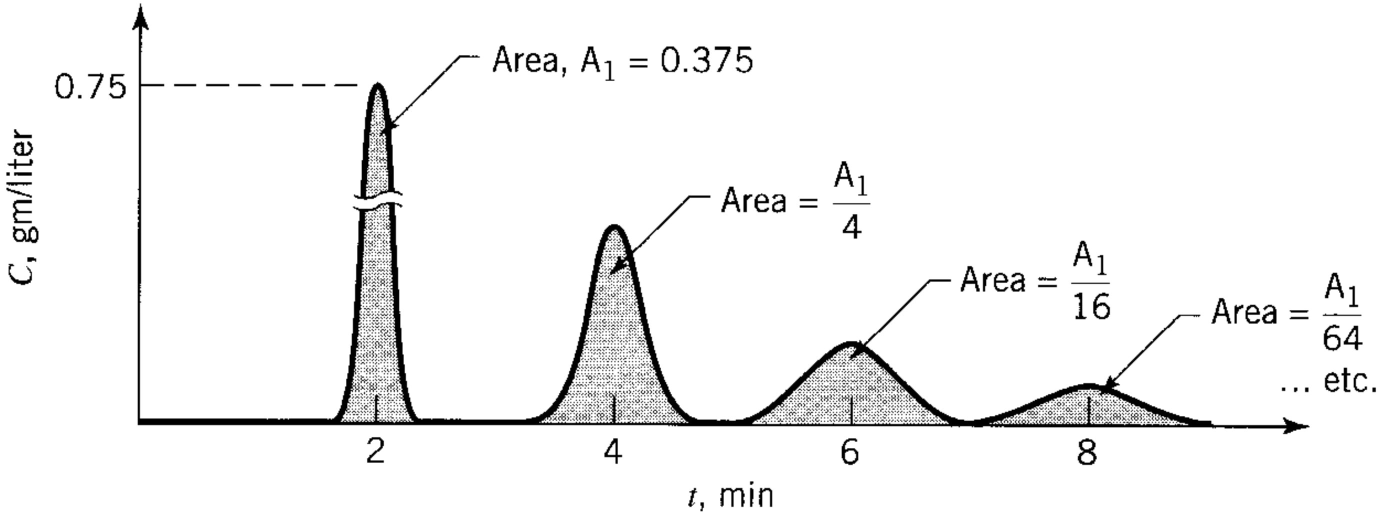


Figure E11.2*a*

SOLUTION

(a) Check the material balance against the tracer curve. From the material balance, Eq. 3, we should have

$$\text{Area} = \frac{M}{v} = \frac{150\ \text{gm}}{5\ \text{liters/s}} = 30\,\frac{\text{gm}\cdot\text{s}}{\text{liter}} = 0.5\,\frac{\text{gm}\cdot\text{min}}{\text{liter}}$$

From the tracer curve

$$\text{Area} = A_1\left(1 + \frac{1}{4} + \frac{1}{16} + \cdots\right) = 0.375\left(\frac{4}{3}\right) = 0.5\,\frac{\text{gm}\cdot\text{min}}{\text{liter}}$$

These values agree. The results are consistent. **(a)**

(b) For the liquid, Eq. 4 gives

$$\bar{t}_l = \frac{\int tC\,dt}{\int C\,dt} = \frac{1}{0.5}\left[2A_1 + 4\times\frac{A_1}{4} + 6\times\frac{A_1}{16} + 8\times\frac{A_1}{64} + \cdots\right] = 2.67\ \text{min}$$

Thus the liquid volume in the vessel is

$$V_l = \bar{t}_l v_l = 2.67(5\times 60) = 800\ \text{liters}$$

and the volume fraction of phases is

$$\left.\begin{aligned} \text{Fraction of liquid} &= \frac{800}{860} = 93\% \\ \text{Fraction of gas} &= 7\% \end{aligned}\right\} \qquad \textbf{(b)}$$

(c) Finally, from Eq. 5 we find the **E** curve, or

$$\mathbf{E} = \frac{C_{\text{pulse}}}{M/v} = \frac{0.75}{0.5}\,\mathrm{C} = 1.5\,\mathrm{C}$$

Thus the **E** curve for the liquid is as shown in Fig. E11.2*b*. **(c)**

(d) The vessel has a strong recirculation of liquid, probably induced by the rising bubbles. **(d)**

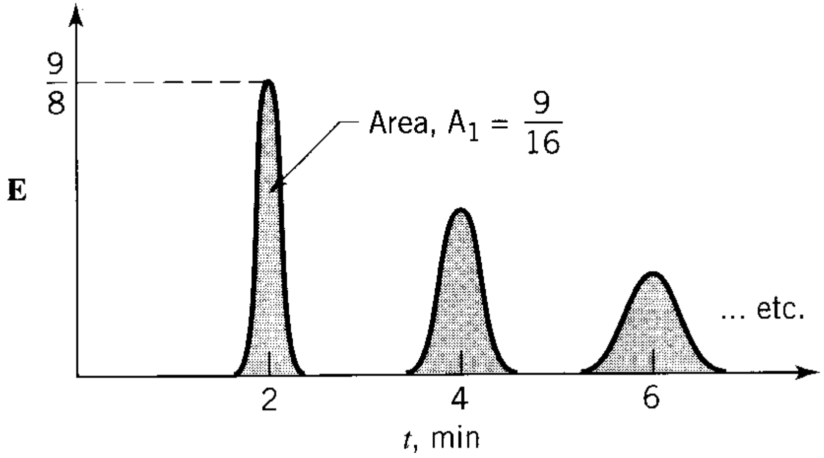
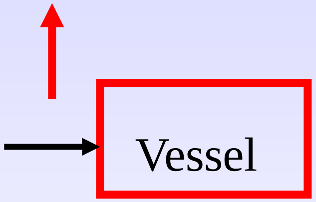


Figure E11.2*b*

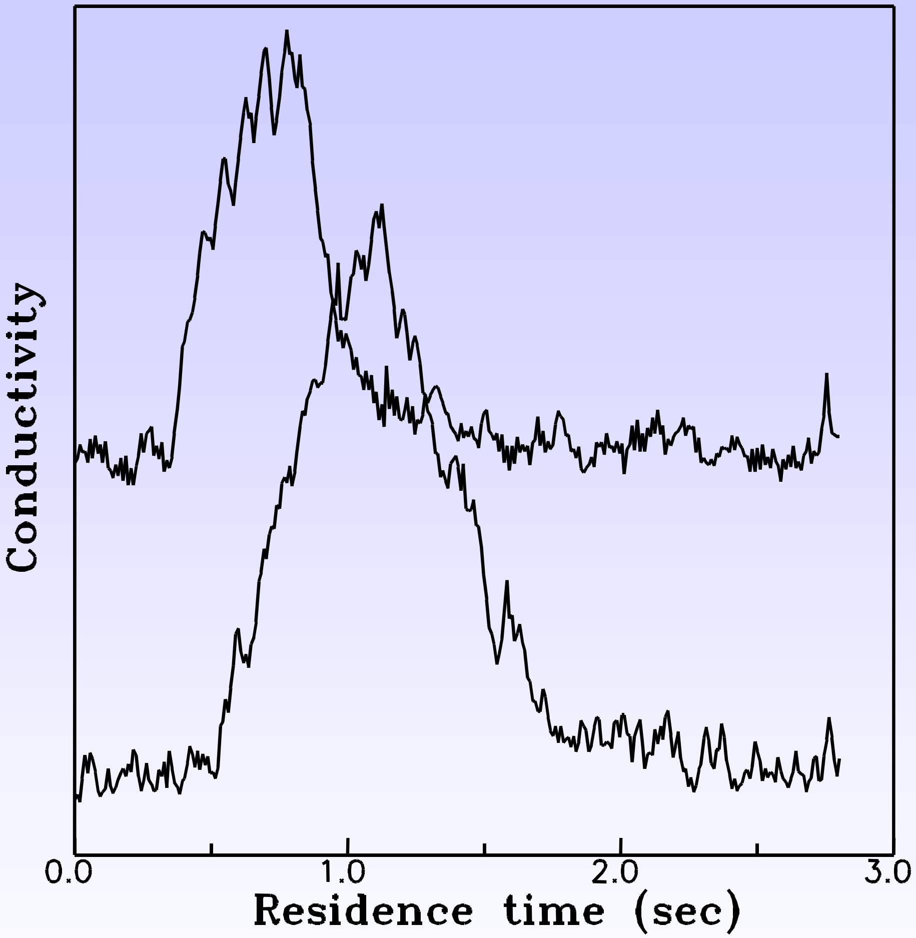
- The Convolution Integral
- In passing through a vessel the C_{in} signal will be modified to give an output signal C_{out} vs. t.



E curve of a rotating packed bed

upper: inlet

lower: outlet



The problem is knowing C_{in} and E, to find C_{out}

- From the figure, we may write

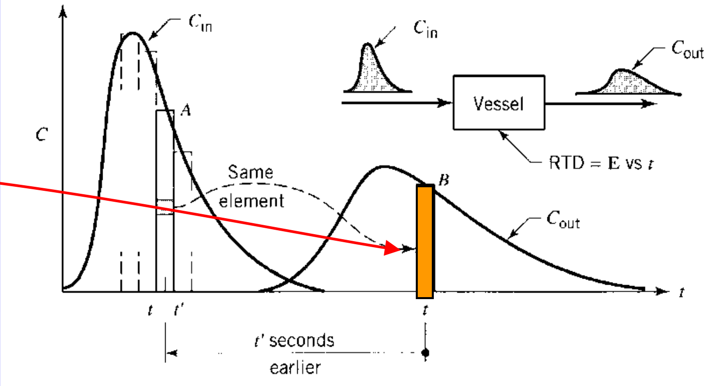


Figure 11.15 Sketch showing derivation of the convolution integral.

$$\begin{pmatrix}\underline{\text{tracer leaving}}\\ \text{in rectangle B}\end{pmatrix} = \begin{pmatrix}\text{All the tracer entering } t' \text{ seconds earler}\\ \text{than t and staying for time } t' \text{ in the vessel}\end{pmatrix}$$

or

$$\begin{pmatrix}\text{tracer leaving}\\ \text{in rectangle B}\end{pmatrix} = \sum_{\substack{\text{all rectangle}\\ \text{A which enter}\\ \text{earler than}\\ \text{time t}}} \begin{pmatrix}\text{tracer in}\\ \text{rectangle}\\ \text{A}\end{pmatrix}\begin{pmatrix}\text{fraction of tracer in A}\\ \text{which stays for about}\\ t' \text{ seconds in the vessel}\end{pmatrix}$$

t’ is a coordinate, not a constant!

- Taking limit, we obtain

$$C_{out}(t) = \int_0^t C_{in}(t-t')E(t')dt' \qquad or$$

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

Briefly :

$$C_{out} = E * C_{in} \qquad or \qquad C_{out} = C_{in} * E$$

The definition of convolution integral

$$\psi(t) \equiv \int_a^b f(t-x)g(x)dx \equiv \int_a^b g(t-x)f(x)dx$$

$$f * g \equiv g * f \qquad f * (g * h) \equiv (f * g) * h \equiv f * g * h$$

$$f * (g + h) \equiv f * g + f * h$$

Application of These Tools

Two Problems--Convolution and Deconvolution

Knowing C_{in} and E find C_{out}

--convolution;

Knowing C_{in} and C_{out}, find E

--deconvolution--illustrated by following Chapter

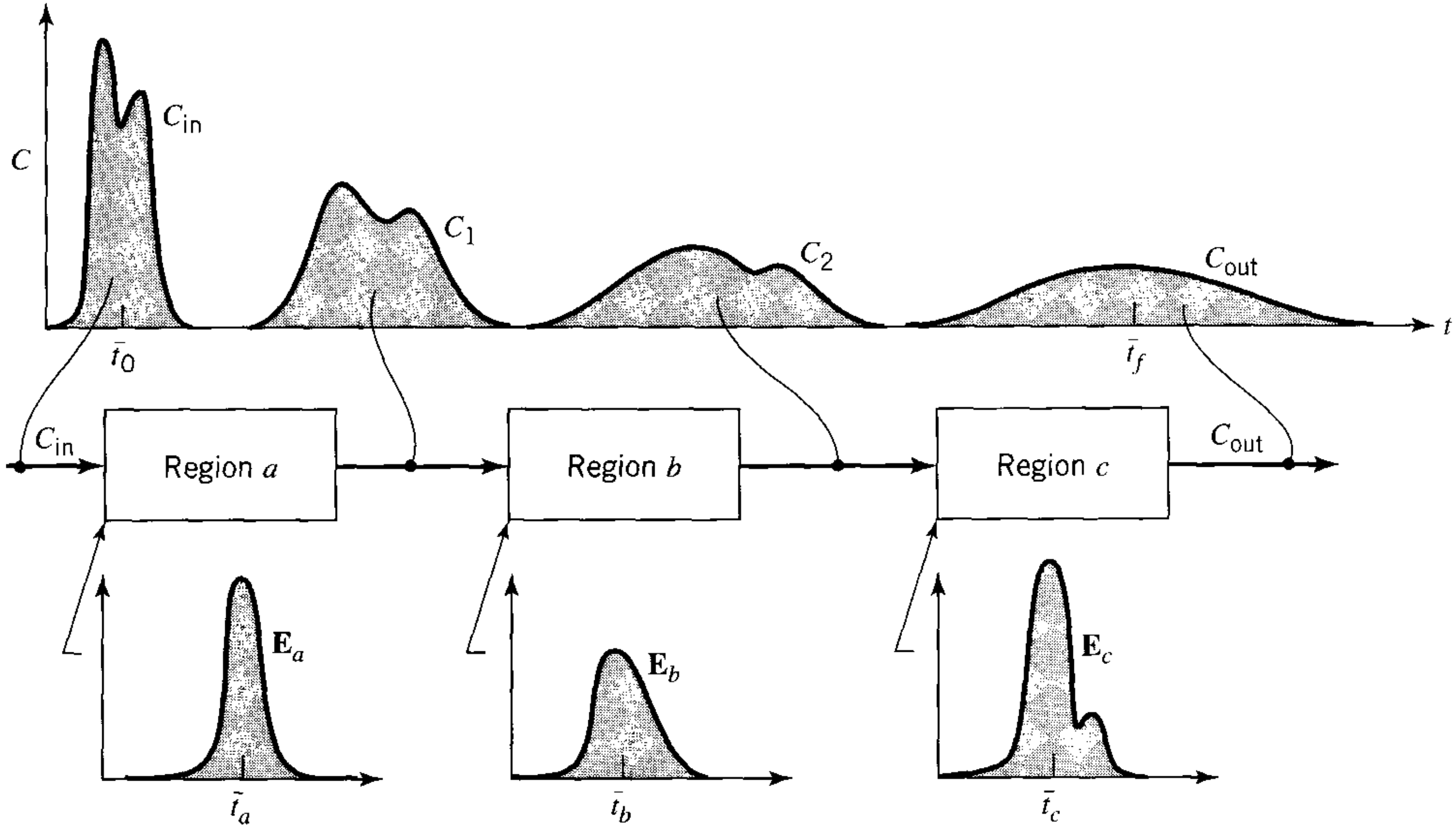


Figure 11.16 Modification of an input tracer signal C_{in} on passing through three successive regions.

$$C_1 = C_{in} * E_a \qquad C_2 = C_1 * E_b \qquad C_{out} = C_2 * E_c$$

$$C_{out} = C_{in} * E_a * E_b * E_c$$

EXAMPLE 11.3 CONVOLUTION

Let us illustrate the use of the convolution equation, Eq. 10, with a very simple example in which we want to find C_{out} given C_{in} and the **E** curve for the vessel, as shown in Fig. E11.3*a*.

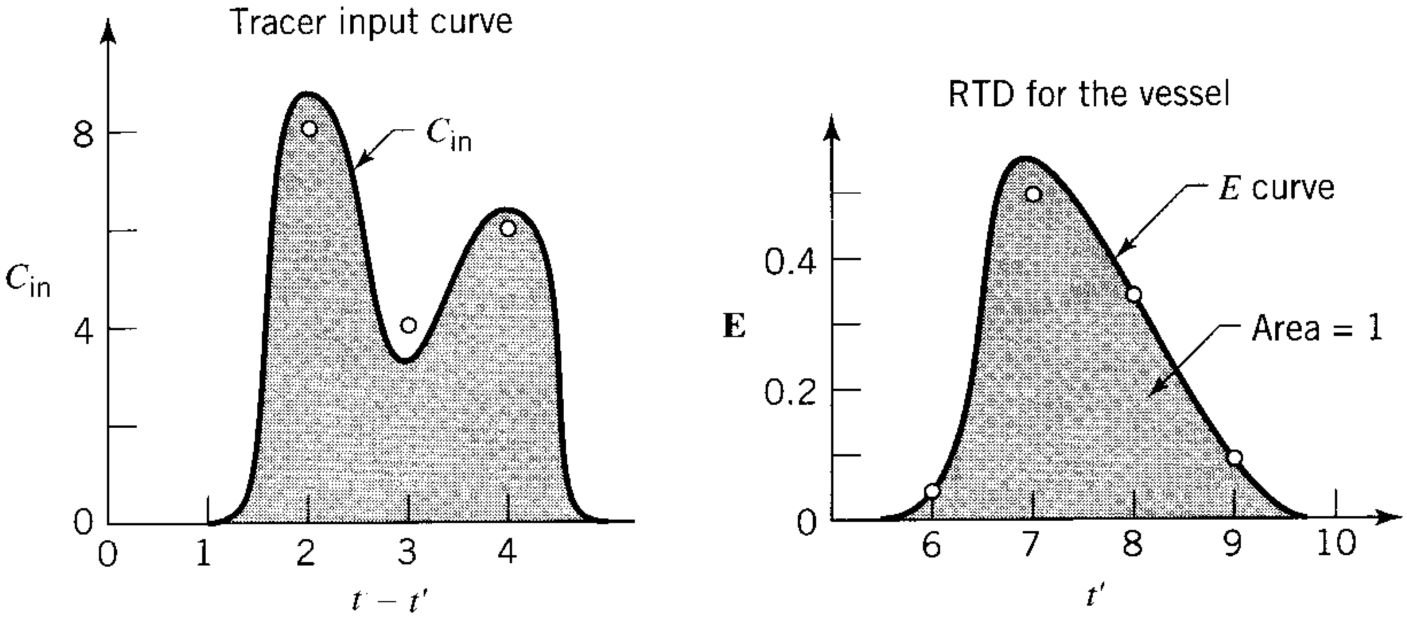


Figure E11.3*a*

SOLUTION

First of all, take 1 min time slices. The given data are then

$t - t'$	C_{in}
0	0
1	0
2	8
3	4
4	6
5	0

t'	**E**
5	0
6	0.05
7	0.50
8	0.35
9	0.10
10	0

Note: The area under the **E** curve is unity.

Now the first bit of tracer leaves at 8 min, the last bit at 13 min. Thus, applying the convolution integral, in discrete form, we have

t	C_{out}
7	$0 = 0$
8	$8 \times 0.05 = 0.4$
9	$8 \times 0.5 + 4 \times 0.05 = 4.2$
10	$8 \times 0.35 + 4 \times 0.5 + 6 \times 0.05 = 5.1$
11	$8 \times 0.10 + 4 \times 0.35 + 6 \times 0.5 = 5.2$
12	$4 \times 0.10 + 6 \times 0.35 = 2.5$
13	$6 \times 0.10 = 0.6$
14	$= 0$

$$C_{out}(t)$$

$$= \int_0^t C_{in}(t-t')E(t')dt'$$

$$= \sum_0^t C_{in}(t-t')E(t')\Delta t'$$

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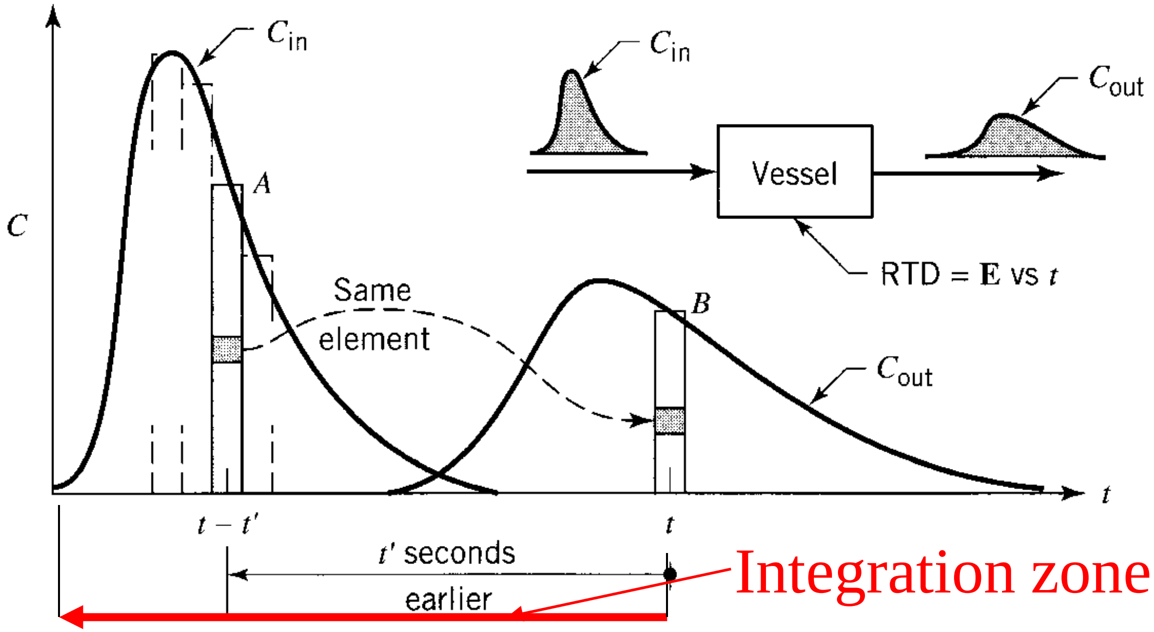

Integration zone

	t’=0		t’=6 E(6)=0.05	t’=7 E(7)=0. 5	t’=8 E(8)=0.35	t’=9 E(9)=0.1	t’=10 E(10)=0	
C(7)=	Cin(7-0)E(0)+	……+	Cin(7-6)E(6)+	Cin(7-7)E(7)				
			0 x 0.05	0 x 0.5				0
C(8)=	Cin(8-0)E(0)+	……+	Cin(8-6)E(6)+	Cin(8-7)E(7)+	Cin(8-8)E(8)			
			8 x 0.05	0 x 0.5				0.4
C(9)=	Cin(9-0)E(0)+	……+	Cin(9-6)E(6)+	Cin(9-7)E(7)+	Cin(9-8)E(8)+	Cin(9-9)E(9)		
			4 x 0.05+	8 x 0.5	0 x 0.35			4.2
C(10)=	Cin(10-0)E(0)+	……+	Cin(10-6)E(6)+	Cin(10-7)E(7)+	Cin(10-8)E(8)+	Cin(10-9)E(9)+	Cin(10-10)E(10)	
			6 x 0.05+	4 x 0.5+	8 x 0.35	0 x 0.1		5.1
C(11)=	Cin(11-0)E(0)+	……+	Cin(11-6)E(6)+	Cin(11-7)E(7)+	Cin(11-8)E(8)+	Cin(11-9)E(9)+	Cin(11-10)E(10)+	
			0 x 0.05	6 x 0.5+	4 x 0.35+	8 x 0.1	0 x 0	5.2
C(12)=	Cin(12-0)E(0)+	……+	Cin(12-6)E(6)+	Cin(12-7)E(7)+	Cin(12-8)E(8)+	Cin(12-9)E(9)+	Cin(12-10)E(10)+	
				0 x 0.5	6 x 0.35+	4 x 0.1	8 x 0	2.5
C(13)=	Cin(13-0)E(0)+	……+	Cin(13-6)E(6)+	Cin(13-7)E(7)+	Cin(13-8)E(8)	Cin(13-9)E(9)+	Cin(13-10)E(10)+	
				0 x 0.5	0 x 0.35	6 x 0.1	4 x 0	0.6
C(14)=	Cin(14-0)E(0)+	……+	Cin(14-6)E(6)+	Cin(14-7)E(7)+	Cin(14-8)E(8)+	Cin(14-9)E(9)+	Cin(14-10)E(10)+	
				0 x 0.5	0 x 0.35	0 x 0.1	6 x 0	0

The C_{in}, **E**, and C_{out} curves, in discrete and in continuous form, are shown in Fig. E11.3*b*. Note that the area under the C_{out} curve equals the area under the C_{in} curve.

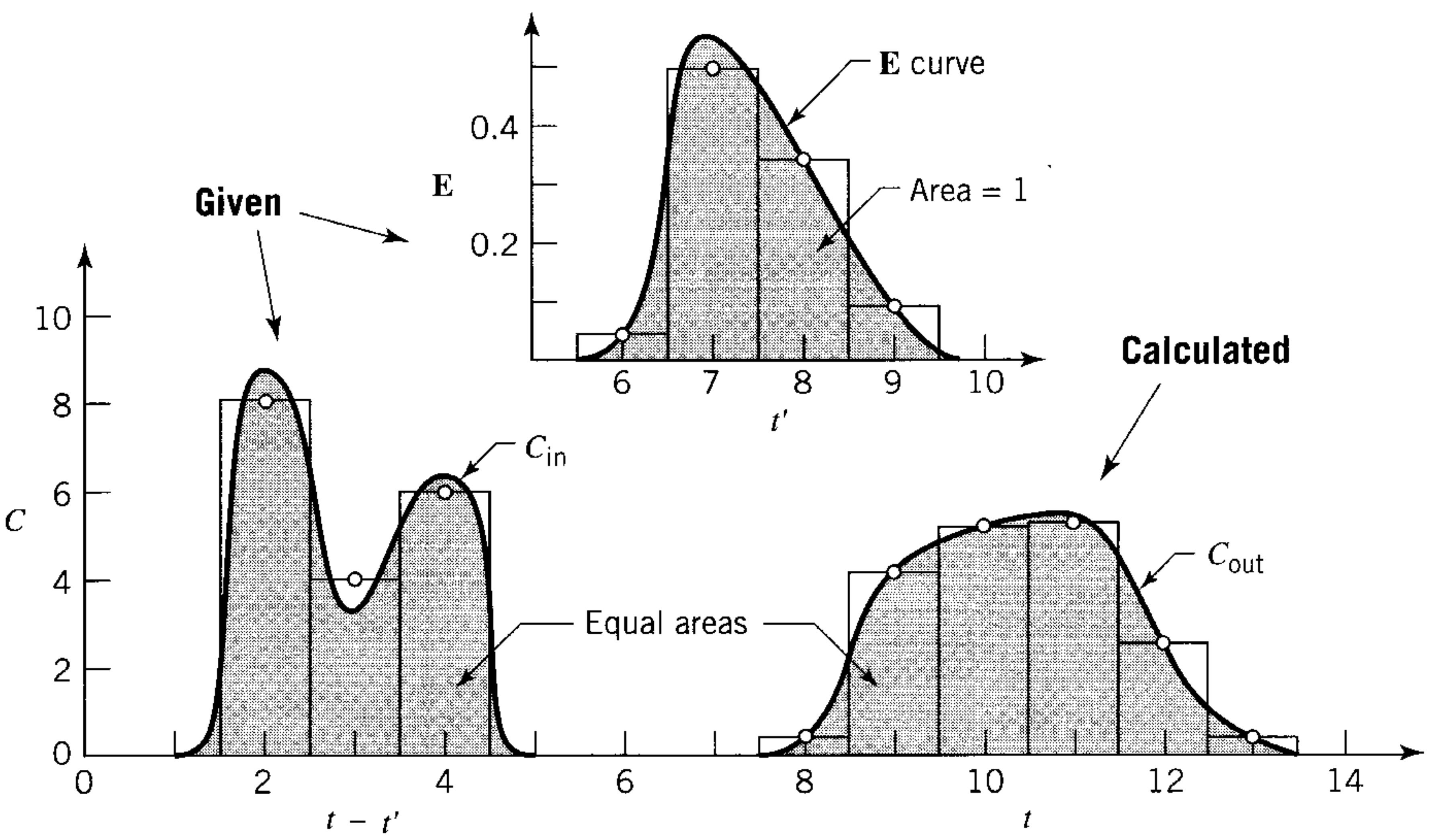

Figure E11.3*b*

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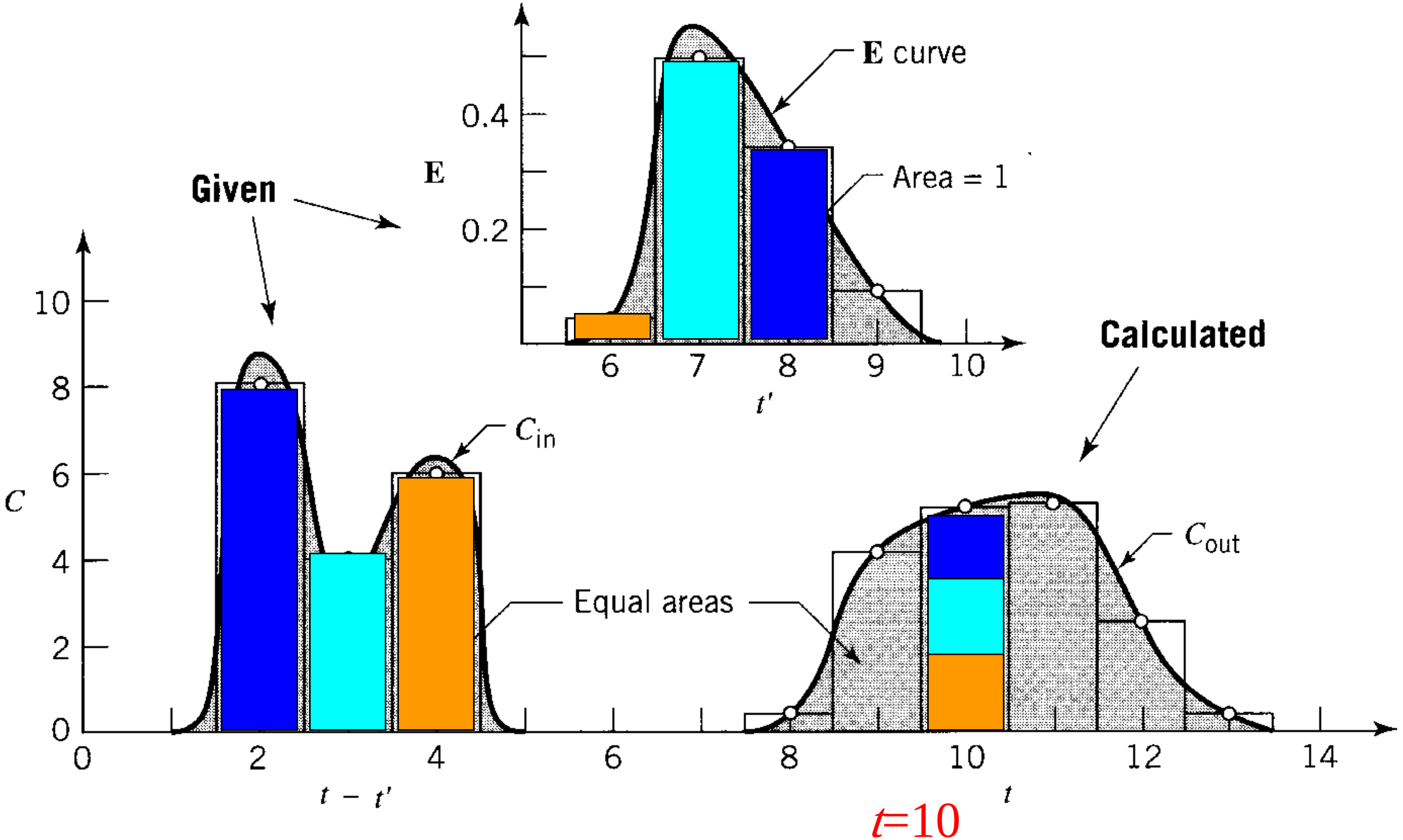

Figure E11.3*b*

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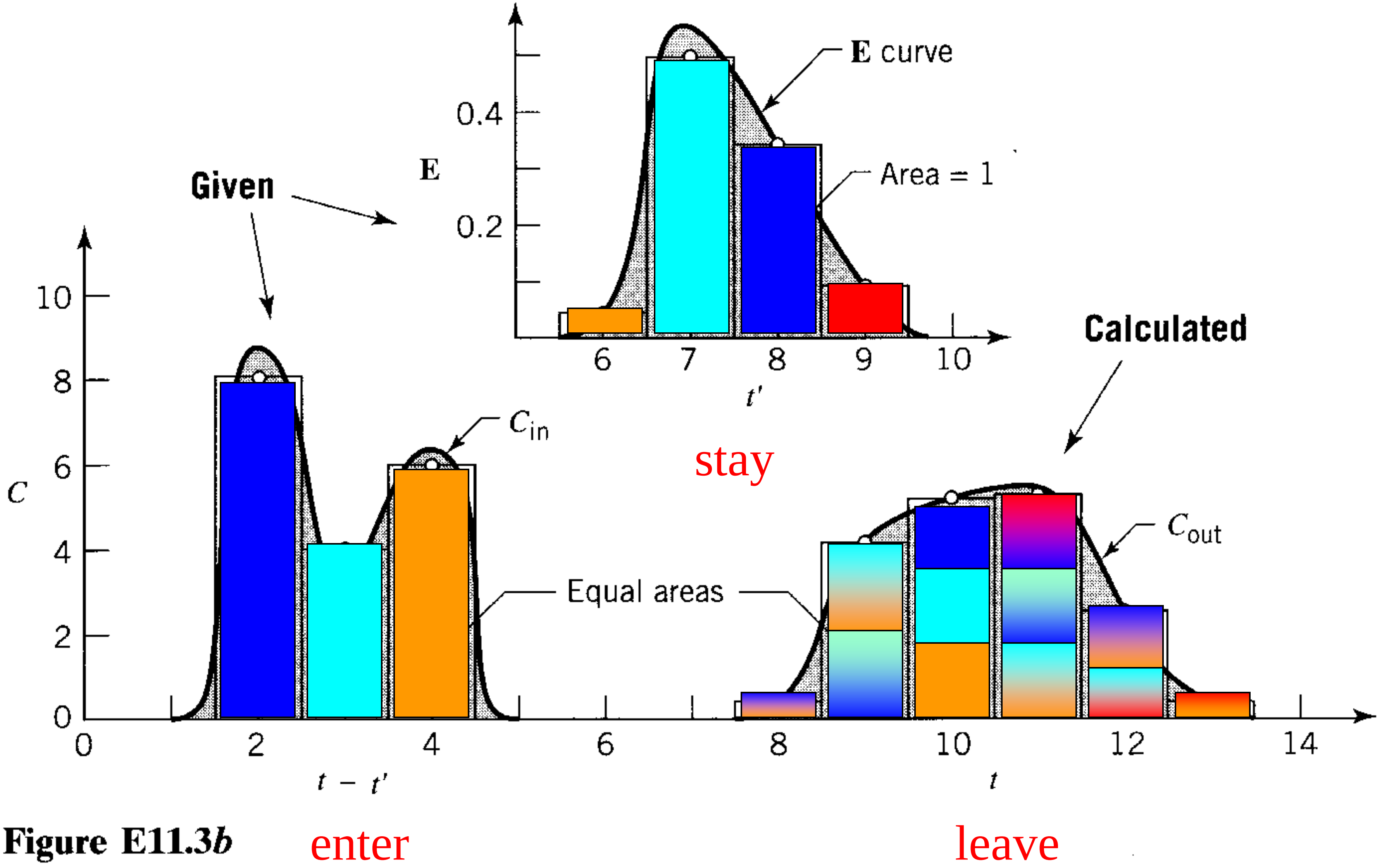

Figure E11.3*b*

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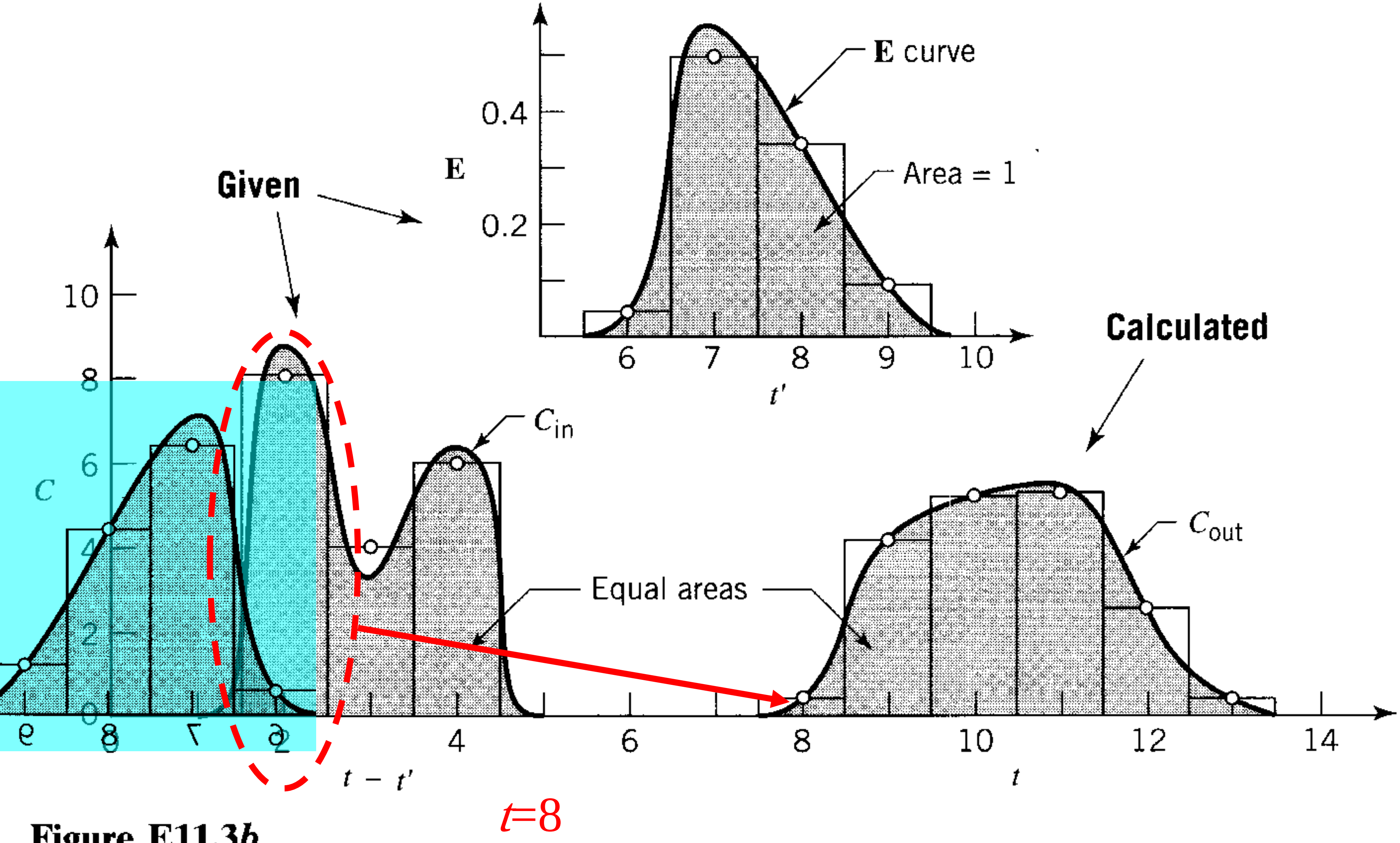

Figure E11.3*b*

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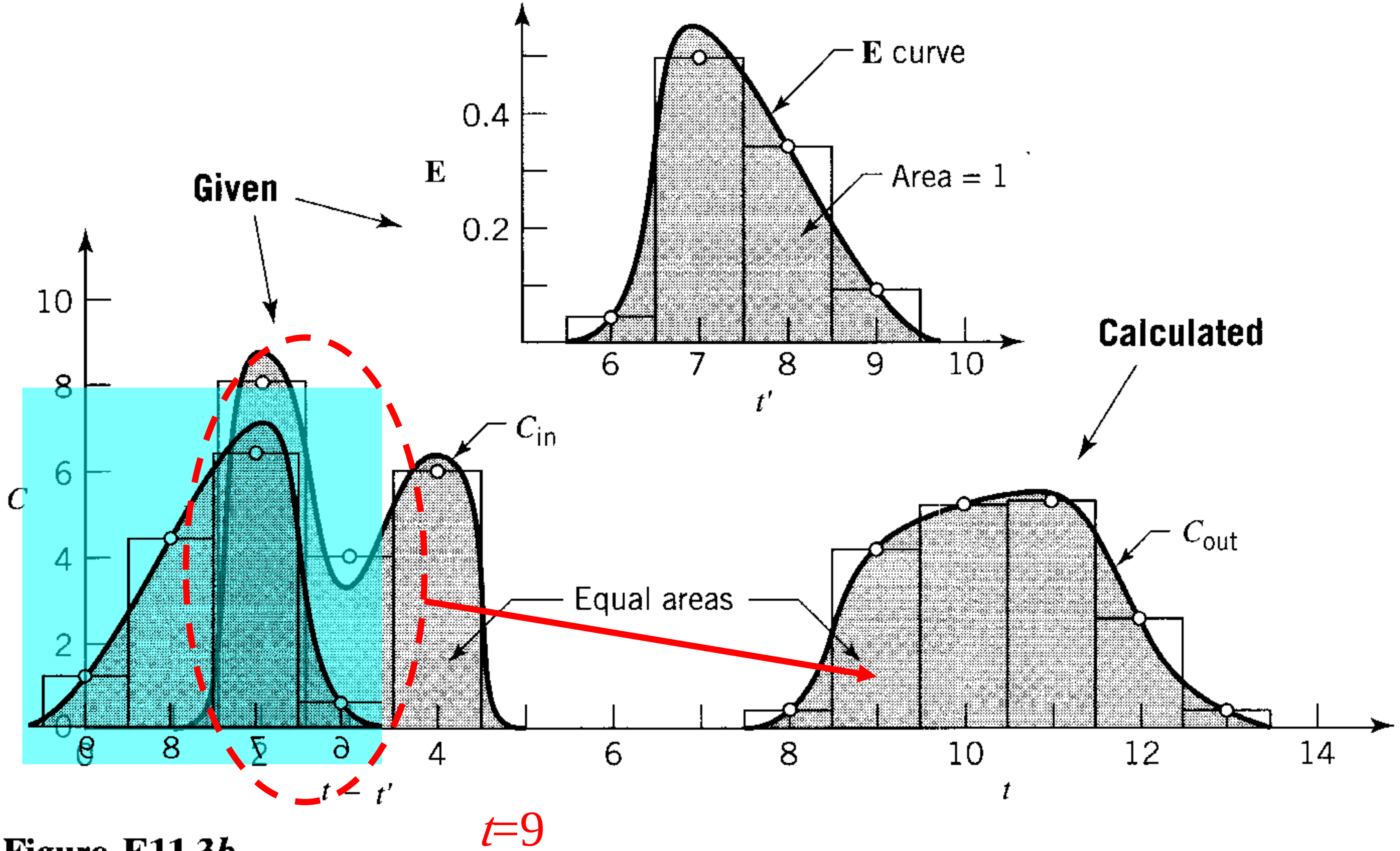

Figure E11.3*b*

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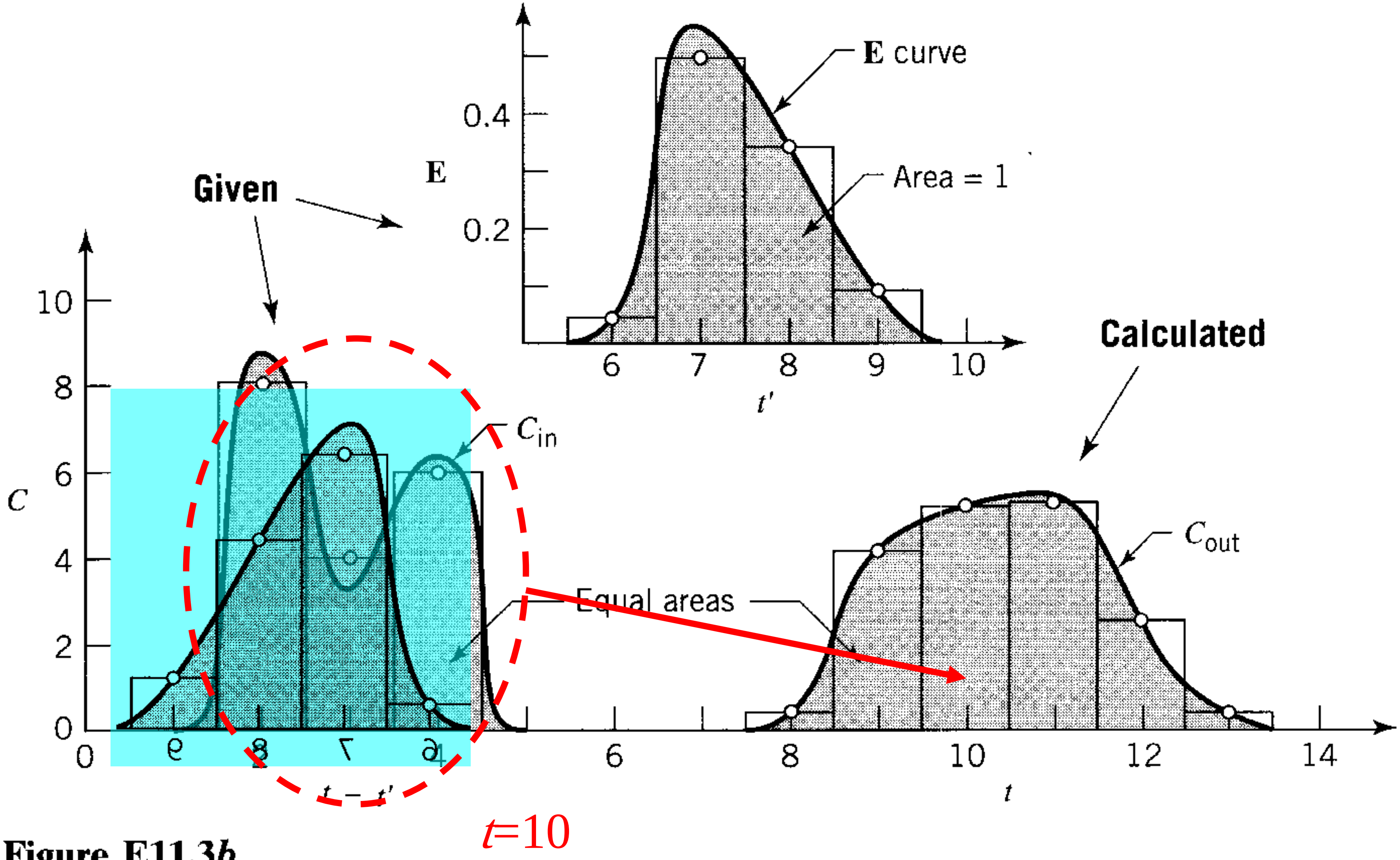

Figure E11.3*b*

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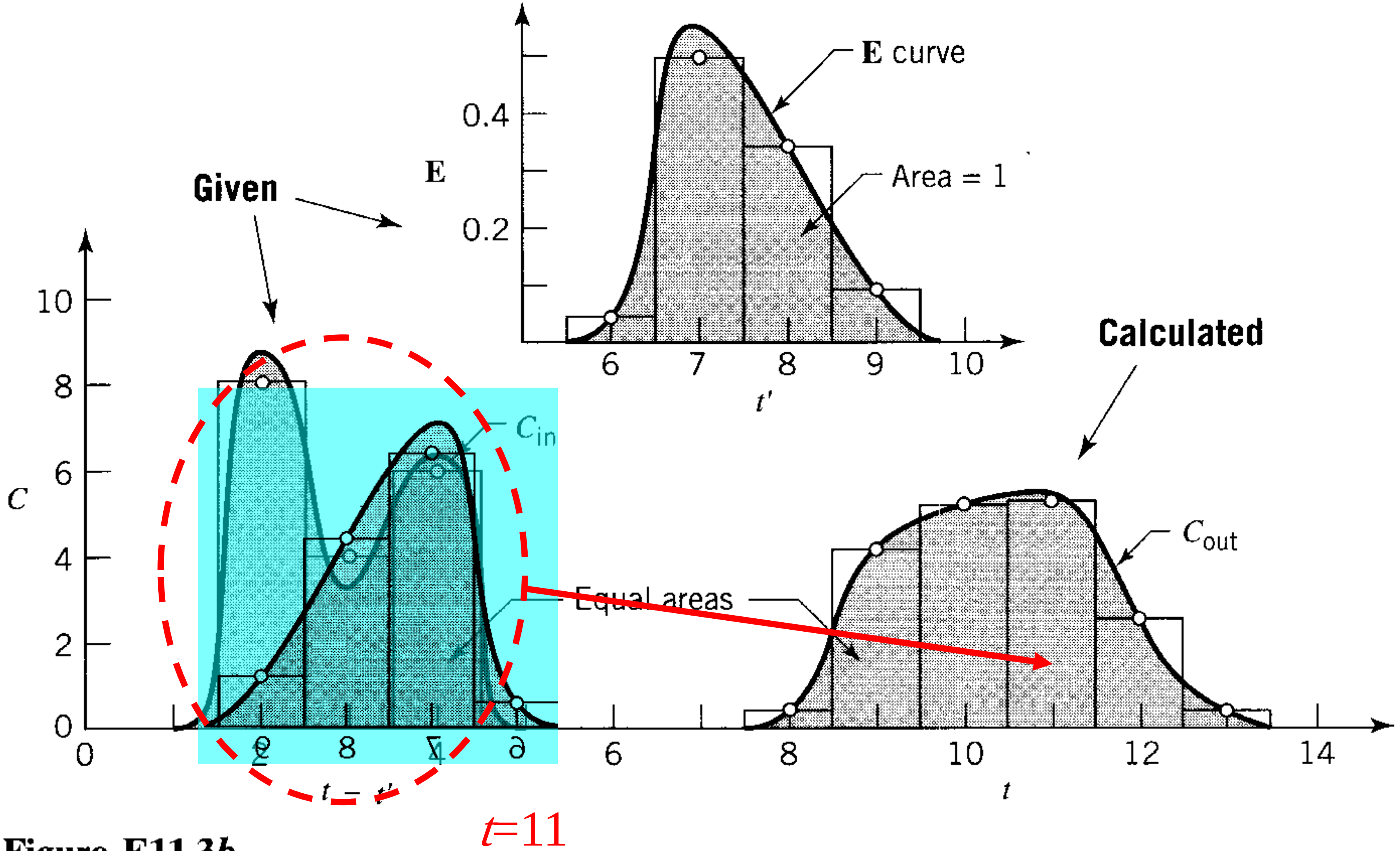

Figure E11.3b

The C_{in}, **E**, and C_{out} curves, in discrete and in continuous form, are shown in Fig. E11.3*b*. Note that the area under the C_{out} curve equals the area under the C_{in} curve.

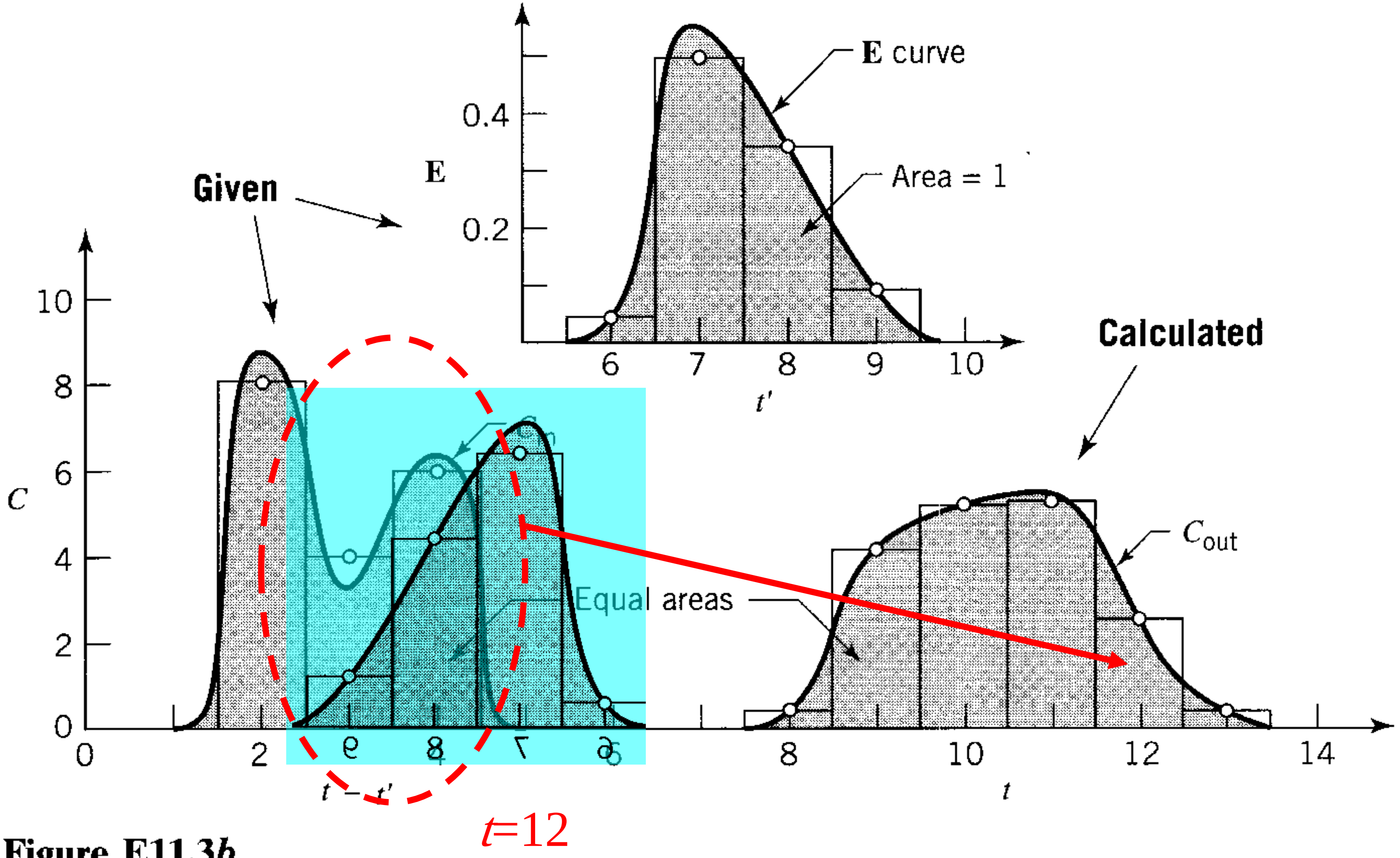

Figure E11.3*b*

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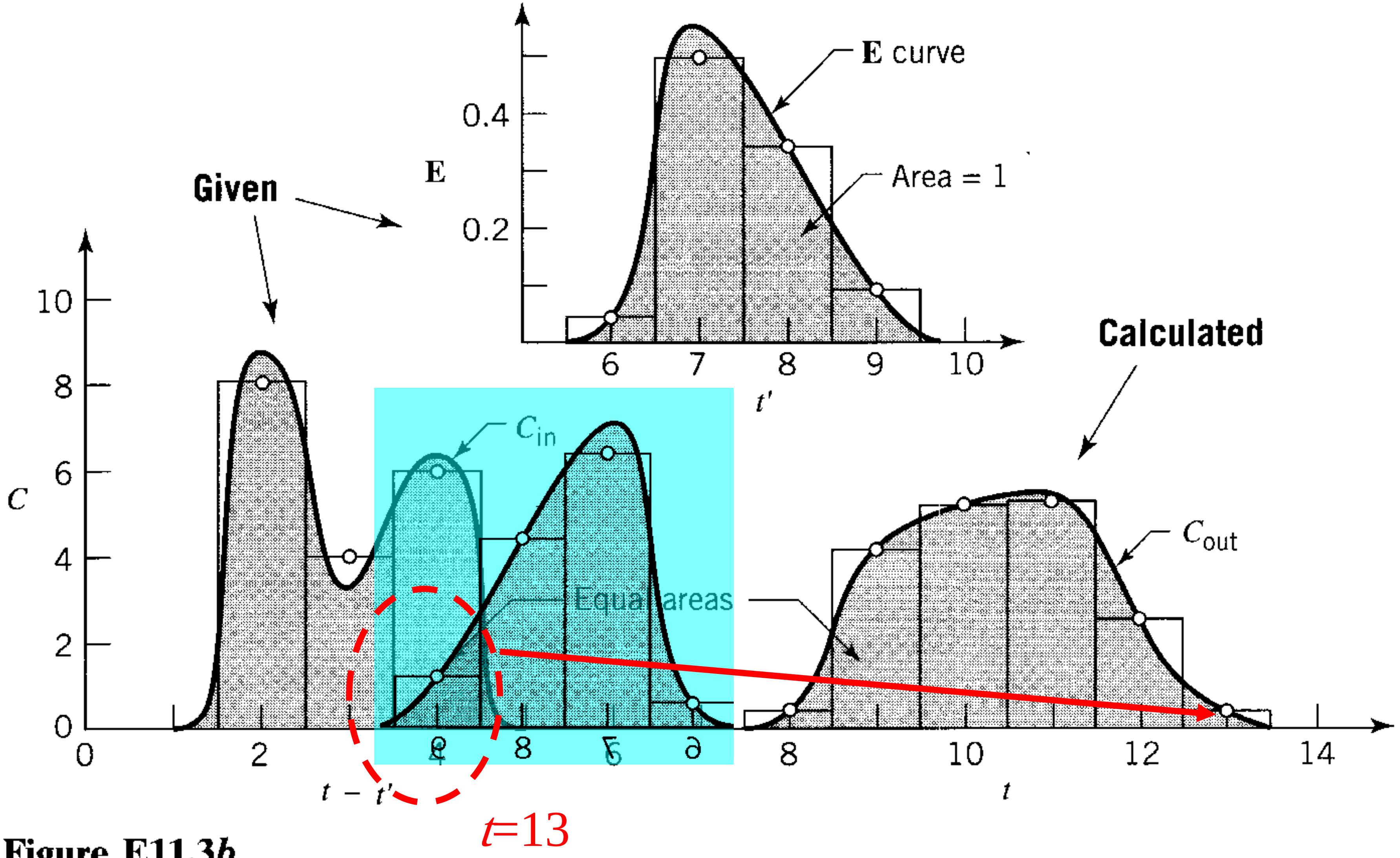


Figure E11.3*b*

11.2 Conversion in Non-ideal Flow Reactor

- To evaluate reactor behavior in general we have to know four factors:
- 1 the kinetics of the reaction
- 2 the RTD of fluid in the reactor
- 3 The earliness or lateness of fluid mixing in the reactor--discuss in Chapter 16 in detail
- 4 whether the fluid is a micro or macro fluid

- For a microfluid, proceeding a nth-order reaction, it is different by early and late mixing.

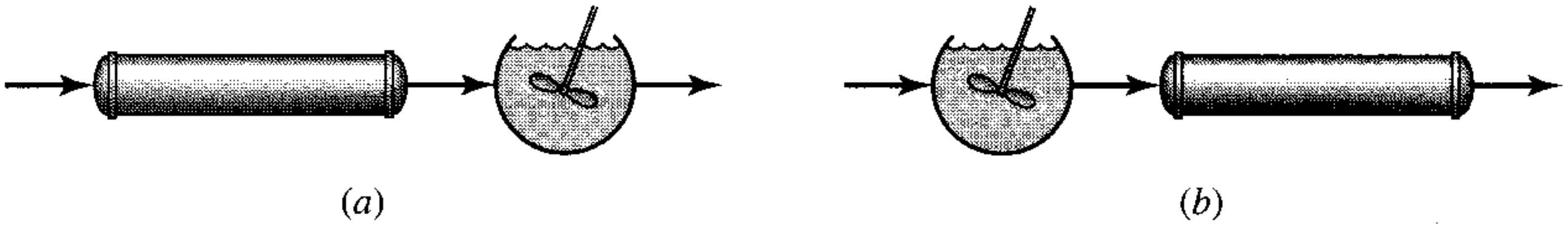
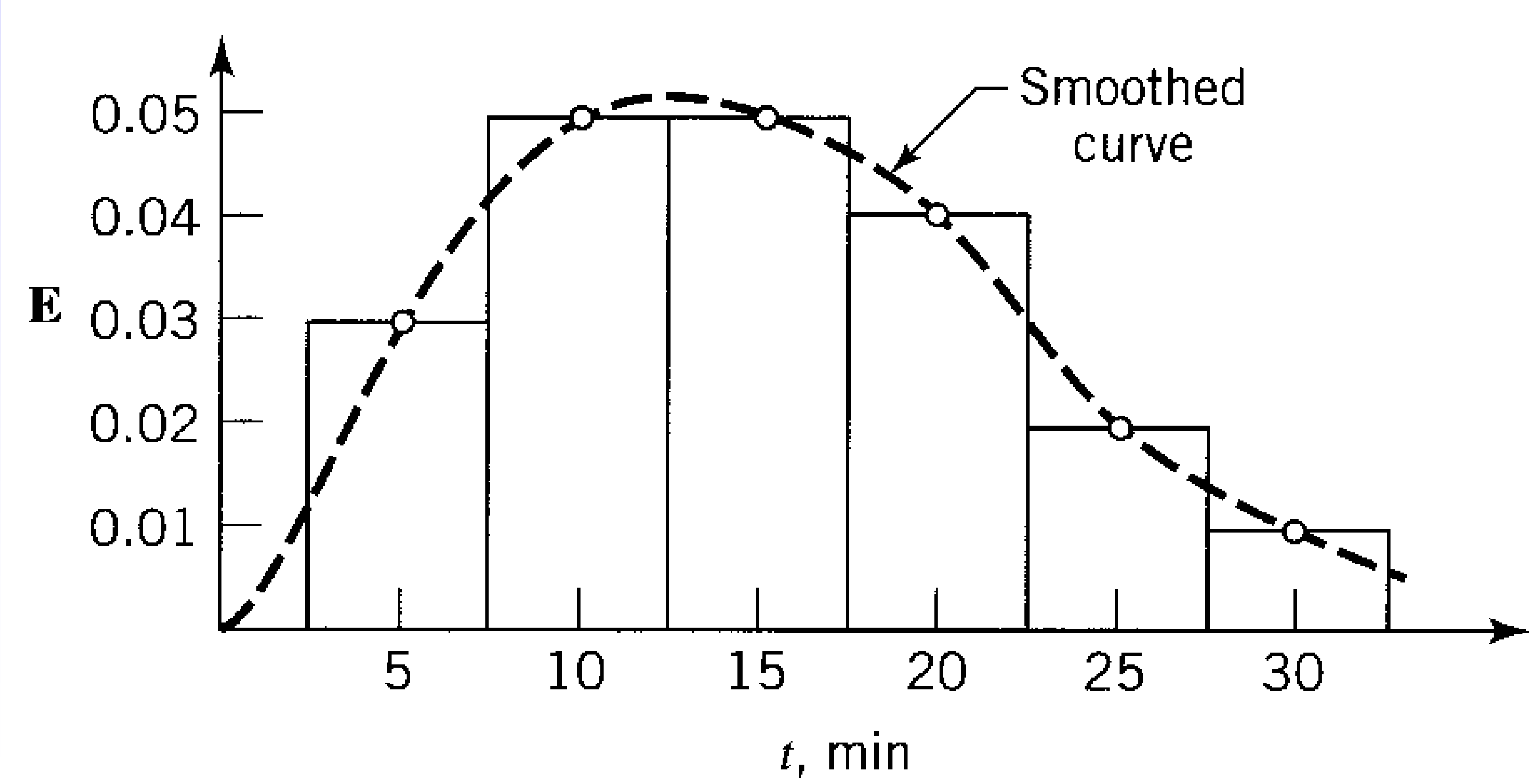

(*a*) (*b*)

Figure 11.17 This shows the latest and the earliest mixing we can have for a given RTD.

- Late mixing favors reaction where n>1
- Early mixing favors reaction where n<1

- For a macrofluid, imagine little clumps of fluid staying for different lengths of time in the reactor(given by the E function). Each clumps reacts away as a little batch reactor, thus fluid elements will have different composition. So the mean composition in the exit stream will have to account for these two factors, the kinetics and the RTD.

$$\begin{pmatrix}\text{mean concentration}\\ \text{of reactant}\\ \text{in exit stream}\end{pmatrix} = \sum_{\substack{\text{all elements}\\ \text{of exit stream}}} \begin{pmatrix}\text{concentration of}\\ \text{reactant remaining}\\ \text{in an element of}\\ \text{age between t}\\ \text{and } t + dt\end{pmatrix} \begin{pmatrix}\text{fraction of exit}\\ \text{stream which is}\\ \text{of age between t}\\ \text{and } t + dt\end{pmatrix}$$



In symbols

$$\left(\frac{\overline{C}_A}{C_{A0}}\right)_{\text{at exit}} = \int_0^{\infty} \left(\frac{C_A}{C_{A0}}\right)_{\left(\substack{\text{For an element or little} \\ \text{batch of fluid of age t}}\right)} E\,dt$$

$$\overline{X}_A = \int_0^{\infty} \left(X_A\right)_{\text{element}} E\,dt$$

$$\left(\frac{\overline{C}_A}{C_{A0}}\right)_{\text{at exit}} = \sum_{\substack{\text{all age} \\ \text{intevals}}} \left(\frac{C_A}{C_{A0}}\right)_{\text{element}} E\Delta t$$

$$\text{for first - order reaction}\left(\text{n} = 1\right) \qquad \left(\frac{C_A}{C_{A0}}\right)_{\text{element}} = e^{-kt}$$

$$n = 2 \qquad \left(\frac{C_A}{C_{A0}}\right)_{\text{element}} = \frac{1}{1 + kC_{A0}t}$$

……

XAMPLE 11.4 CONVERSION IN REACTORS HAVING NON-IDEAL FLOW

The vessel of Example 11.1 is to be used as a reactor for a liquid decomposing with rate

$$-r_A = kC_A, \qquad k = 0.307\ \text{min}^{-1}$$

Find the fraction of reactant unconverted in the real reactor and compare this with the fraction unconverted in a plug flow reactor of the same size.

SOLUTION

For the *plug flow reactor* with negligible density change we have

$$\tau = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} = -\frac{1}{k}\int_{C_{A0}}^{C_A}\frac{dC_A}{C_A} = \frac{1}{k}\ln\frac{C_{A0}}{C_A}$$

and with τ from Example 11.1

$$\frac{C_A}{C_{A0}} = e^{-k\tau} = e^{-(0.307)(15)} = e^{-4.6} = \underline{\underline{0.01}}$$

Thus the fraction of reactant unconverted in a plug flow reactor equals 1.0%.

For the *real reactor* the fraction unconverted, given by Eq. 13 for macrofluids, is found in Table E11.4. Hence the fraction of reactant unconverted in the real reactor

$$\frac{C_A}{C_{A0}} = \underline{\underline{0.047}}$$

Table E11.4

t	$\mathbf{E}$	kt	e^{-kt}	$e^{-kt}\mathbf{E}\,\Delta t$
5	0.03	1.53	0.2154	$(0.2154)(0.03)(5) = 0.0323$
10	0.05	3.07	0.0464	0.0116
15	0.05	4.60	0.0100	0.0025
20	0.04	6.14	0.0021	0.0004
25	0.02	7.68	0.005	0.0001
30	0.01	9.21	0.0001	0
given				$\frac{C_A}{C_{A0}} = \sum e^{-kt}\mathbf{E}\,\Delta t = \underline{\underline{0.0469}}$

From the table we see that the unconverted material comes mostly from the early portion of the **E** curve. This suggests that channeling and short-circuiting can seriously hinder attempts to achieve high conversion in reactors.

Note that since this is a first-order reaction we can treat it as a microfluid, or a macrofluid, whatever we wish. In this problem we solved the plug flow case as a microfluid, and we solved the nonideal case as a macrofluid.

EXAMPLE 11.5 *REACTION OF A MACROFLUID*

Dispersed noncoalescing droplets ($C_{A0} = 2$ mol/liter) react ($A \rightarrow R$, $-r_A = kC_A^2$, $k = 0.5$ liter/mol·min) as they pass through a contactor. Find the average concentration of A remaining in the droplets leaving the contactor if their RTD is given by the curve in Fig. E11.5.

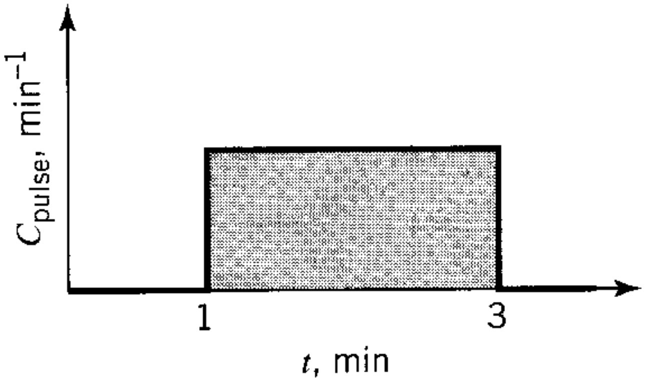


Figure E11.5

SOLUTION

Equation 13 is the pertinent performance equation. Evaluate terms in this expression. For

$$-r_A = kC_A^2, \qquad k = 0.5 \text{ liter/mol} \cdot \text{min}$$

The batch equation from Chapter 3 is

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + kC_{A0}t} = \frac{1}{1 + 0.5(2)t} = \frac{1}{1 + t}$$

With **E** = 0.5 for 1 < t < 3, Eq. 13 becomes

$$0.5 = \frac{1}{3-1}$$

$$\frac{\overline{C}_A}{C_{A0}} = \int_0^\infty \left(\frac{C_A}{C_{A0}}\right)_{\text{batch}} \mathbf{E}\, dt = \int_1^3 \frac{1}{1+t} \cdot (0.5)dt = 0.5 \ln 2 = 0.347$$

So

$$\overline{X}_A = 1 - 0.347 = 0.653, \qquad \text{or} \qquad \underline{\underline{65\%}}$$