1

Non-ideal Flow and Reactor Characterization

Summary of Residence Time Distribution Properties and Most Important Models

Residence Time Distribution

In a reactor, C(t) is obtained by injecting pulse of tracer. From that:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t) \cdot dt}$$
$$\int_0^\infty E(t)dt = 1$$
$$\int_0^t E(t)dt = F(t)$$
$$I(t) = 1 - F(t)$$

Total amount of tracer injected is:

$$M_0 = Q_0 \int_0^\infty C(t) \mathrm{d}t$$

In a step tracer run:

$$E(t) = \frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{C(t)}{C_0} \right]_{\mathrm{step input}}$$

Mean residence time:

$$t_m = \frac{\int_0^\infty t \cdot C(t) dt}{\int_0^\infty C(t) dt} = \int_0^\infty t \cdot E(t) dt = \int_0^\infty t \cdot E(t) dt$$

Variance of the residence time distribution (RTD):

$$\sigma^2 = \int_0^\infty \left(t - t_m\right)^2 \cdot E(t) \mathrm{d}t$$

The square root of the variance, σ , is called standard deviation. Average residence time:

$$\overline{t} = \frac{V}{Q}$$

Problem Solving in Chemical Reactor Design, First Edition. Juan A. Conesa. © 2025 WILEY-VCH GmbH. Published 2025 by WILEY-VCH GmbH.

RTD in Ideal Reactors

For the plug flow reactor (PFR):

$$E(t) = \delta(t - \overline{t})$$

For the continuous stirred tank reactor (CSTR):

$$E(t) = \frac{1}{\bar{t}} \cdot \exp(-t/\bar{t})$$

Tanks-in-series (TIS) Model

$$E(t) = \frac{t^{n_t - 1}}{(n_t - 1)! \overline{t}_i^{n_t}} \cdot \exp\left(-\frac{t}{\overline{t}_i}\right)$$
$$\sigma^2 = \frac{t_m^2}{n_t}$$
$$n_t = \frac{t_m^2}{\sigma^2}$$

Dispersion Model

$$Bo = \frac{D_e}{u \cdot L}$$

Bo < 0.01

$$E = \frac{1}{\overline{t} \cdot \sqrt{4 \cdot \pi \cdot Bo}} \cdot \exp\left[-\frac{\left(1 - \frac{t}{\overline{t}}\right)^2}{4 \cdot Bo}\right]$$
$$t_m = \overline{t} = \frac{V}{Q}$$
$$\sigma^2 = 2 \cdot Bo$$

Bo > 0.01, Closed-Closed Recipient

E(t) is only integrable by numerical methods.

$$\overline{t} = t_m$$

 $\left(\frac{\sigma}{t_m}\right)^2 = 2 \cdot \text{Bo} - 2 \cdot \text{Bo}^2 \cdot \left[1 - \exp\left(-\frac{1}{\text{Bo}}\right)\right]$

. .

Bo > 0.01, Open-Open Recipient

$$E = \frac{1}{\sqrt{4 \cdot \pi \cdot \operatorname{Bo} \cdot t/\overline{t}}} \cdot \exp\left[-\frac{\left(1 - \frac{t}{\overline{t}}\right)^2}{4 \cdot \operatorname{Bo} \cdot t/\overline{t}}\right]$$
$$t_m = \overline{t} \cdot (1 + 2 \cdot \operatorname{Bo})$$

$$\left(\frac{\sigma}{t_m}\right)^2 = 2 \cdot \mathrm{Bo} + 8 \cdot \mathrm{Bo}^2$$

Designing E_1 to the E(t) given by the first expression (valid for Bo < 0.01) and E_2 to the one predicted by the open-open (o–o) assumption, the differences between these RTDs are small at low Bo, but at a high Bo number, E_1 is not valid (for more details, consult spreadsheet "dispersion model Bo fitting.xls"):



Problem 1.1 A solution of potassium permanganate (KMnO₄) was rapidly injected into a water stream flowing through a circular tube at a linear velocity of 35.70 cm/s. A photoelectric cell located 2.74 m downstream from the injection point was utilized to monitor the local concentration of KMnO₄.

- (a) By using the given effluent $KMnO_4$ concentrations, calculate the average residence time of the fluid as well as the variance, E(t), F(t), and I(t).
- (b) Determine the number of ideal tanks (n_t) , the variance, the dispersion number, and the Peclet number.

Time (s)	KMnO ₄ concentration
0.0	0.0
2.0	11.0
4.0	53.0
6.0	64.0
8.0	58.0
10.0	48.0
12.0	39.0
14.0	29.0
16.0	22.0
18.0	16.0
20.0	11.0
22.0	9.0
24.0	7.0
26.0	5.0
28.0	4.0
30.0	2.0
32.0	2.0
34.0	2.0
36.0	1.0
38.0	1.0
40.0	1.0
42.0	1.0

Solution to Problem 1.1

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

t (s)	C(t)	C(t)dt	E(t)	t∙E(t)	t·E(t)·∆t	$(t-t_m)^2 \cdot E(t)$	$(t-t_m)^2 \cdot E(t) \cdot \Delta t$	F(t)	l(t)
0	0	0	0.000	0.000	0.000	0.000	0.000	0.000	1.000
2	11	11	0.014	0.029	0.029	1.149	1.149	0.029	0.971
4	53	64	0.069	0.275	0.304	3.345	4.494	0.166	0.834
6	64	117	0.083	0.498	0.773	2.055	5.399	0.332	0.668
8	58	122	0.075	0.602	1.100	0.666	2.721	0.482	0.518
10	48	106	0.062	0.623	1.224	0.059	0.725	0.607	0.393
12	39	87	0.051	0.607	1.230	0.053	0.112	0.708	0.292
14	29	68	0.038	0.527	1.134	0.344	0.397	0.783	0.217
16	22	51	0.029	0.457	0.983	0.720	1.065	0.840	0.160
18	16	38	0.021	0.374	0.830	1.024	1.744	0.882	0.118
20	11	27	0.014	0.285	0.659	1.162	2.186	0.911	0.089
22	9	20	0.012	0.257	0.542	1.419	2.581	0.934	0.066
24	7	16	0.009	0.218	0.475	1.540	2.959	0.952	0.048
26	5	12	0.006	0.169	0.387	1.464	3.004	0.965	0.035
28	4	9	0.005	0.145	0.314	1.504	2.968	0.975	0.025
30	2	6	0.003	0.078	0.223	0.939	2.443	0.981	0.019
32	2	4	0.003	0.083	0.161	1.147	2.086	0.986	0.014
34	2	4	0.003	0.088	0.171	1.375	2.522	0.991	0.009
36	1	3	0.001	0.047	0.135	0.812	2.187	0.994	0.006
38	1	2	0.001	0.049	0.096	0.947	1.759	0.996	0.004
40	1	2	0.001	0.052	0.101	1.093	2.040	0.999	0.001
42	1	2	0.001	0.054	0.106	1.248	2.341		
$\Sigma(C$	(t)dt) =	= 771		$t_m =$	10.98 s	$\sigma^2 =$	$46.88 {\rm s}^2$		

(a) To solve this problem, we should use a spreadsheet. First, data given in the statement are introduced, and then we should do the following calculations:

We can calculate time increment as the difference between time in two experimental data; in the third column, concentration and time increment are multiplied. For a better calculation, instead of calculating $C(t) \cdot \Delta t$ for each time directly, we can use the average value of C(t) between two consecutive data. This is called Simpson's rule for evaluating areas graphically. The sum of the values in this column would give the area of the C(t) curve, so in the fourth column, the following relationship is applied to calculate E(t):

$$E(t) = \frac{C(t)}{\int_0^\infty C(t) \cdot dt} = \frac{C(t)}{771}$$

In the next columns, the average value of E(t) between two consecutive data is multiplied by time, by time increment, and the sum would represent mean time, as we have:

$$t_m = \int_0^\infty t \cdot E(t) dt = \sum_{\text{all points}} t \cdot E(t) \cdot \Delta t = 10.98 \text{ s}$$

In a similar way, variance is calculated:

$$\sigma^{2} = \sum_{\text{all points}} (t - t_{m})^{2} \cdot E(t) \cdot \Delta t = 46.88 \text{ s}^{2}$$

Finally, we can calculate F(t) and I(t) according to their definitions:

$$F(t) = \sum_{\text{all points at time} < t} E(t) \cdot \Delta t$$
$$I(t) = 1 - F(t)$$

We can check the form of the graphs showing the distributions:







(b) From the calculated parameters, it is easy to find the number of tanks in the TIS model:

$$\sigma^{2} = \frac{t_{m}^{2}}{n_{t}}$$
$$n_{t} = \frac{t_{m}^{2}}{\sigma^{2}} = \frac{10.98^{2}}{46.88} = 2.57 \text{ tanks}$$

For the dispersion model to be applied, first we should assume Bo < 0.01, and then:

$$\sigma^2 = 2 \cdot \text{Bo}$$

We obtain $Bo = 11.24 \gg 0.01$, so this assumption is not valid. Assuming now Bo > 0.01 and closed-closed recipient:

$$\left(\frac{\sigma}{t_m}\right)^2 = 2 \cdot \text{Bo} - 2 \cdot \text{Bo}^2 \cdot \left[1 - \exp\left(-\frac{1}{\text{Bo}}\right)\right]$$

From that:

$$\frac{46.88}{10.98^{2}} = 2 \cdot \operatorname{Bo} - 2 \cdot \operatorname{Bo}^{2} \cdot \left[1 - \exp\left(-\frac{1}{\operatorname{Bo}}\right)\right]$$

and we obtain Bo = 0.2413, and Pe = 1/Bo = 4.14. On the other hand, if an o-o recipient is assumed:

$$\left(\frac{\sigma}{t_m}\right)^2 = 2 \cdot \mathrm{Bo} + 8 \cdot \mathrm{Bo}^2$$

Obtaining Bo = 0.127 and Pe = 7.85.

For checking which one of the conditions is fulfilled, data about average time in the recipient is needed in order to test if the equation $t_m = \bar{t} \cdot (1 + 2 \cdot Bo)$ is satisfied.

$$\bar{t} = \frac{\text{Length}}{\text{Linear velocity}} = \frac{274 \text{ cm}}{35.70 \frac{\text{cm}}{\text{s}}} = 7.67 \text{ s}$$

So, we have that:

10.98 = 7.67 (1 + 2Bo)

Obtaining Bo = 0.215. This difference between t_m and \bar{t} indicates that probably the recipient is open.

Problem 1.2 An experiment to characterize a tubular reactor was conducted using a technique in which a tracer is continuously fed into the system. At a specific time, the tracer supply is halted. From this point onward, the exit signal is recorded, resembling what can be termed a "decreasing step input" (or negative step). In this experiment, the following data were obtained:

t(min)	0	1	2	4	6	7	8	10
C(g/l)	0.5	0.5	0.5	0.4	0.1	0	0	0

- (a) Calculate the RTD of this reactor.
- (b) What fraction of the fluid spends more than 3 minutes in the reactor? Make a plot of the procedure.
- (c) What fraction of the fluid spends between 3 and 4 minutes in the reactor?

Solution to Problem 1.2

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) Following this procedure, the exit signal will be related to the cumulative RTD of the system, F(t), but the actual function obtained is the internal age function, I(t). In the spreadsheet, we can do the following calculation:

t (min)	C (g/l)	C/C _{max}	l(t)	F(t)	$E(t) = \Delta F / \Delta t$
0	0.5	1	1	0	0.00
1	0.5	1	1	0	0.00
2	0.5	1	1	0	0.10
4	0.4	0.8	0.8	0.2	0.30
6	0.1	0.2	0.2	0.8	0.20
7	0	0	0	1	0.00
8	0	0	0	1	0.00
10	0	0	0	1	

In the table, I(t) is derived directly from the data, and:

F(t) = 1 - I(t)

For the calculation of E(t), a numerical derivative is done:

$$E(t) = \frac{F^{t+1} - F}{\Delta t}$$

Obtaining:



(b) For calculating the fraction of fluid that spends a time in the reactor, we use the definition of *E*(*t*):

Fluid passing more than 3 minutes $= f_{>3} = \int_{3}^{\infty} E(t) dt$

This integration can be done numerically, in increments:

 $f_{>3} = E(3) \cdot \Delta t + E(4) \cdot \Delta t + E(5) \cdot \Delta t + E(6) \cdot \Delta t + E(7) \cdot \Delta t$

where Δt is obviously 1 minute. Graphically, the approximation of the integral would be the following:



Obviously, this is a rough approximation. A better approximation would involve using smaller time increments, but this is not possible with the obtained data.

More precision is obtained if average value of the E(t) function is used, so:

$$f_{>3} = \frac{E(3) + E(4)}{2} \cdot \Delta t + \frac{E(4) + E(5)}{2} \cdot \Delta t + \frac{E(5) + E(6)}{2} \cdot \Delta t + \frac{E(6) + E(7)}{2} \cdot \Delta t + \frac{E(7) + E(8)}{2} \cdot \Delta t$$
$$= \left(\frac{E(3)}{2} + E(4) + E(5) + E(6) + E(7) + \frac{E(8)}{2}\right) \cdot \Delta t = 0.85$$

In this situation, we are doing the following approximation in the graph:



(c) If we look for the fraction of fluid passing between 3 and 4 minutes:

$$f_{3-4} = \int_{3}^{4} E(t) dt = E(3) \cdot \Delta t + E(4) \cdot \Delta t = 0.5$$

Problem 1.3 This problem involves a reactor with a flow rate of 10 l/min. Concentration measurements were taken at the outlet during a pulse test at various time intervals. The data obtained are as follows:

<i>t</i> (min)	$c imes 10^5$ (g/l)	<i>t</i> (min)	$c imes 10^5$ (g/l)
0	0	15	238
0.4	329	20	136
1.0	622	25	77
2.0	812	30	44
3	831	35	25
4	785	40	14

t (min)	c × 10 ⁵ (g/l)	<i>t</i> (min)	<i>c</i> × 10⁵ (g/l)
5	720	45	8
6	650	50	5
8	523	60	1
10	418		

- (a) Determine the volume of the reactor and plot the functions E(t), F(t), and I(t) as a function of time.
- (b) Determine the number of tanks required to model the reactor using a TIS system.
- (c) Calculate the Peclet number (Pe) if the reactor is modeled using a dispersion model.

Solution to Problem 1.3

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) This problem is quite similar to Problem 1.1. In a spreadsheet, we calculate:

<i>t</i> (min)	C(t) (g/l)	C(t)·∆t	E(t)	$t \cdot E(t) \cdot \Delta t$	$(t-t_m)^2 \cdot E(t)$	$(t-t_m)^2 \cdot E(t) \cdot \Delta t$
0	0	0	0.0000	0	0	0
0.4	$3.29 \cdot 10^{-3}$	$1.32 \cdot 10^{-3}$	0.0368	0.0059	3.4842	1.3937
1	$6.22 \cdot 10^{-3}$	$3.73 \cdot 10^{-3}$	0.0697	0.0418	5.7993	3.4796
2	$8.12 \cdot 10^{-3}$	$8.12 \cdot 10^{-3}$	0.0909	0.1819	6.0023	6.0023
3	$8.31 \cdot 10^{-3}$	$8.31 \cdot 10^{-3}$	0.0931	0.2792	4.7237	4.7237
4	$7.85 \cdot 10^{-3}$	$7.85 \cdot 10^{-3}$	0.0879	0.3516	3.2975	3.2975
5	$7.20 \cdot 10^{-3}$	$7.20 \cdot 10^{-3}$	0.0806	0.4031	2.1175	2.1175
6	$6.50 \cdot 10^{-3}$	$6.50 \cdot 10^{-3}$	0.0728	0.4367	1.2383	1.2383
8	$5.23 \cdot 10^{-3}$	$1.05 \cdot 10^{-2}$	0.0586	0.9371	0.2644	0.5288
10	$4.18 \cdot 10^{-3}$	$8.36 \cdot 10^{-3}$	0.0468	0.9362	0.0007	0.0015
15	$2.38 \cdot 10^{-3}$	$1.19 \cdot 10^{-2}$	0.0267	1.9989	0.6335	3.1675
20	$1.36 \cdot 10^{-3}$	$6.80 \cdot 10^{-3}$	0.0152	1.5230	1.4853	7.4263
25	$7.70 \cdot 10^{-4}$	$3.85 \cdot 10^{-3}$	0.0086	1.0779	1.9080	9.5401
30	$4.40 \cdot 10^{-4}$	$2.20 \cdot 10^{-3}$	0.0049	0.7391	1.9464	9.7322
35	$2.50 \cdot 10^{-4}$	$1.25 \cdot 10^{-3}$	0.0028	0.4899	1.7324	8.6618
40	$1.40 \cdot 10^{-4}$	$7.00 \cdot 10^{-4}$	0.0016	0.3136	1.3993	6.9965
45	$8.00 \cdot 10^{-5}$	$4.00 \cdot 10^{-4}$	0.0009	0.2016	1.0896	5.4482
50	$5.00 \cdot 10^{-5}$	$2.50 \cdot 10^{-4}$	0.0006	0.1400	0.8903	4.4515
60	$1.00 \cdot 10^{-5}$	$1.00 \cdot 10^{-4}$	0.0001	0.0672	0.2786	2.7857
	$\Sigma(C(t)\mathrm{d}t)$	$= 8.93 \cdot 10^{-2}$	$t_m =$	= 10.12 s	σ^2	$= 80.99 s^2$

We easily obtain:



For calculating the volume of the system, we have:

$$\bar{t} = t_m = \frac{V}{Q}; \quad 10.12 = \frac{V}{10}$$

So the volume is 101.2 l.

(b)

$$n_{\rm t} = \frac{t_m^2}{\sigma^2} = \frac{10.12^2}{80.99} = 1.26 \,{\rm tanks}$$

(c) As in Problem 1.1, we do not know if the recipient is closed or open. Assuming closed-closed condition, we obtain Bo = 1.33 and Pe = 0.75.

Problem 1.4



In the given reactor configurations, where the total volume is represented as $V = V_1 + V_2$, and the ratio V_1/V_2 is imposed, we need to determine the ratio of the volumes V_1/V_2 in the second configuration in order to achieve the same exit conversion, X_{A2} , for both a first-order reaction and a second-order reaction.

Solution to Problem 1.4

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

In the first case:



We can write:

$$X_{\rm A1} = 1 - \exp\left(-k \cdot \frac{V_1}{Q_0}\right)$$

and in the CSTR:

$$\begin{aligned} Q_0 C_{A1} &= (-r_A) V_2 + Q_0 C_{A2} \\ Q_0 C_{A0} (1 - X_{A1}) &= (k \cdot C_{A0} (1 - X_{A2})) \cdot V_2 + Q_0 C_{A0} (1 - X_{A2}) \\ (1 - X_{A1}) &= (k \cdot (1 - X_{A2})) \cdot \frac{V_2}{Q_0} + (1 - X_{A2}) \end{aligned}$$

And solving for X_{A2} :

$$(1 - X_{A2}) = \frac{(1 - X_{A1})}{1 + k \cdot \frac{V_2}{Q_0}} = \frac{\exp\left(-k \cdot \frac{V_1}{Q_0}\right)}{1 + k \cdot \frac{V_2}{Q_0}}$$

In the second configuration:



we have, in the CSTR: $Q_0 C_{A0} = (-r_A)V_2 + Q_0 C_{A1}$ So: $X_{A1} = 1 - \frac{1}{1+k \cdot \frac{V_2}{Q_0}}$. Then, in the PFR:

$$\int_{X_{A1}}^{X_{A2}} \frac{dX_A}{1 - X_A} = k \int_0^{V_1} \frac{dV}{Q_0}$$

that is:

$$\ln\left(\frac{1-X_{A1}}{1-X_{A2}}\right) = k \cdot \frac{V_1}{Q_0}$$

$$1 - X_{A2} = (1 - X_{A1}) \cdot \exp\left(-k \cdot \frac{V_1}{Q_0}\right)$$

$$= \left(1 - \frac{1}{1+k \cdot \frac{V_2}{Q_0}}\right) \cdot \exp\left(-k \cdot \frac{V_1}{Q_0}\right) = \frac{\exp\left(-k \cdot \frac{V_1}{Q_0}\right)}{1+k \cdot \frac{V_2}{Q_0}}$$

We can check that both configurations give the same final conversion.

In the case where a second-order reaction took place, the procedure is similar. In that case, for the first configuration, in the PFR:

$$dn_{A} = Q_{0} \cdot dC_{A} = (r_{A}) \cdot dV = -k \cdot C_{A}^{2} \cdot dV$$
$$-Q_{0} \cdot C_{A0} \cdot dX_{A} = -k \cdot C_{A0}^{2} \cdot (1 - X_{A})^{2} \cdot dV$$

$$\begin{split} &Q_0 \cdot dX_A = k \cdot C_{A0} \cdot (1 - X_A)^2 \cdot dV \\ &\int_0^{X_{A1}} \frac{dX_A}{(1 - X_A)^2} = \int_0^{V_1} k \frac{C_{A0}}{Q_0} dV \\ &- \frac{X_{A1}}{X_{A1} - 1} = k \frac{C_{A0}}{Q_0} V_1 \\ &1 - X_{A1} = \frac{1}{1 + k \cdot C_{A0} \cdot \frac{V_1}{Q_0}} \end{split}$$

and in the CSTR:

$$Q_0 C_{A0}(1 - X_{A1}) = k \cdot C_{A0}^2 (1 - X_{A2})^2 V_2 + Q_0 C_{A0} (1 - X_{A2})^2 V_2$$

So finally:

$$\begin{split} &Q_0 C_{A0} \frac{1}{1 + k \cdot C_{A0} \cdot \frac{V_1}{Q_0}} = k \cdot C_{A0}^2 (1 - X_{A2})^2 V_2 + Q_0 C_{A0} (1 - X_{A2}) \\ &k \cdot C_{A0} (1 - X_{A2})^2 \frac{V_2}{Q_0} + (1 - X_{A2}) - (1 - X_{A1}) = 0 \\ &k \cdot C_{A0} \cdot \overline{t_2} \cdot (1 - X_{A2})^2 + (1 - X_{A2}) - (1 - X_{A1}) = 0 \end{split}$$

This expression is a second-order equation. It is quite complicated to solve the final conversion, but finally, for the first configuration:

$$(1 - X_{A2}) = \frac{-1 + (1 + 4 \cdot k \cdot C_{A0} \cdot \overline{t_2} \cdot (1 - X_{A1}))^{0.5}}{2 \cdot k \cdot C_{A0} \cdot \overline{t_2}}$$

Obviously, the other solution with minus sign does not make sense. In the second configuration, following the same procedure:

$$\begin{aligned} Q_0 C_{A0} &= k \cdot C_{A0}^2 (1 - X_{A1})^2 V_2 + Q_0 C_{A0} (1 - X_{A1}) \\ k \cdot C_{A0} \cdot \overline{t_2} \cdot (1 - X_{A1})^2 + (1 - X_{A1}) - 1 = 0 \\ (1 - X_{A1}) &= \frac{-1 + (1 + 4 \cdot k \cdot C_{A0} \cdot \overline{t_2})^{0.5}}{2 \cdot k \cdot C_{A0} \cdot \overline{t_2}} \end{aligned}$$

and finally, in the PFR:

$$(1 - X_{A2}) = \frac{1 - X_{A1}}{1 + k \cdot C_{A0} \cdot \overline{t_2} + (1 - X_{A1})}$$

We can check the form of the solution by assuming values of the constants. For example, $k \cdot C_{A0} = 0.1 \text{ mol/l} \cdot \text{s}$, $Q_0 = 1 \text{ l/s}$, V = 100 l, and the following graphs can be calculated. As we can check, in any case, the first configuration (PFR + CSTR) gives a higher conversion than the second configuration (CSTR + PFR). In all cases, V_1 refers to the volume of the PFR and V_2 to that of CSTR.



Problem 1.5

(a) Obtain the cumulative probability function for the following data arising from stable operation with concentration of 0.122 M, followed by a step disturbance with C = 0.548 M.

<i>t</i> (s)	10	20	30	45	60	90	120	200	400	1000
$C(\mathbf{M})$	0.126	0.43	0.207	0.314	0.378	0.484	0.505	0.527	0.544	0.547

- (b) Obtain a polynomial for its interpolation, and calculate the average residence time using numerical integration by the method of trapezoids.
- (c) Calculate the average time using the polynomial.

Solution to Problem 1.5

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) The resolution of this problem required a spreadsheet. Let us calculate the E(t) as the derivative of the $C_{\text{step}}(t)$ function, i.e.,

$$E(t) = \frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{C(t)}{C_0} \right]_{\mathrm{step input}} = \frac{1}{C_0} \left(\frac{\Delta C}{\Delta t} \right)_{\mathrm{step}}$$

Furthermore, $C_0 = \sum_{\text{all points}} C(t) \cdot \Delta t$. We can do the following calculation, similar to that presented in Problems 1.1 and 1.3:

Summary of Residence Time Distribution Properties and Most Important Models | 19

t (s)	C _{step} (M)	C(t)∙dt	E(t)	t∙E(t)	t∙E(t)∙dt	$(t-t_m)^2 \cdot E(t)$	$(t-t_m)^2 \cdot E(t) \cdot dt$
10	0.004		0.0002	0.0024		65.133	
20	0.021	1.35	0.0003	0.0055	0.04	71.085	681.09
30	0.085	1.75	0.0004	0.0120	0.09	98.874	849.79
45	0.192	3.91	0.0006	0.0274	0.30	141.053	1799.46
60	0.256	5.19	0.0007	0.0440	0.54	159.384	2253.28
90	0.362	12.93	0.0009	0.0845	1.93	178.663	5070.70
120	0.383	14.84	0.0010	0.1175	3.03	161.660	5104.84
200	0.405	41.28	0.0010	0.2044	12.88	108.806	10818.61
400	0.422	107.10	0.0011	0.4220	62.64	16.824	12 562.99
1000	0.425	327.30	0.0011	1.0608	444.85	238.058	76 464.73
		Sum			$t_m(s)$		σ^2
		515.6375			526.28		115 605.49

Note that the concentration measured has been subtracted from the 0.122 M of the stable operation.

And then:





- (b) The polynomial of the fitting is shown in the previous figure. Using numerical integration of the data, we obtain $t_m = 532.79$ s.
- (c) Using the polynomial shown in the figure, we can do:

$$t_m = \int_0^\infty t \cdot E(t) \mathrm{d}t$$

as:

$$E(t) = \frac{\mathrm{d}F(t)}{\mathrm{d}t} = 2 \cdot 1.437 \cdot 10^{-7} t + 8.898 \cdot 10^{-4}$$
$$t_m = \int_0^\infty t \cdot (2 \cdot 1.437 \cdot 10^{-7} t + 8.898 \cdot 10^{-4}) \cdot \mathrm{d}t$$

This function cannot be integrated because the integral does not converge, as the upper limit is infinity. If we change this limit to, for example, 1000 (high enough to bear in mind all the tracer leaving the system), this can be solved, and:

$$t_m = \int_0^{1000} t \cdot (2 \cdot 1.437 \cdot 10^{-7} t + 8.898 \cdot 10^{-4}) \cdot dt = 540.7 \,\mathrm{s}$$

Problem 1.6 A continuous reactor normally operates with a feed of 50 l/s. Under these conditions, the dynamic data for different pulses presented below were obtained.

- (a) To what type of reactor do these data surely correspond?
- (b) Obtain the residence time distribution.
- (c) Estimate the residence time and the volume of the reactor, and
- (d) Calculate the total mass of the tracer used in the three runs.

		C _{tracer} (mg/l)	
<i>t</i> (s)	Run 1	Run 2	Run 3
0	0.011	0.012	0.001
1	0.553	0.534	0.538
2	0.899	0.907	0.887
3	0.923	0.953	0.934
5	0.860	0.856	0.876
8	0.681	0.723	0.758
12	0.550	0.586	0.585
17	0.413	0.435	0.442
27	0.320	0.331	0.350
38	0.251	0.236	0.276
58	0.162	0.158	0.176
86	0.085	0.103	0.097
130	0.023	0.008	0.015

Solution to Problem 1.6

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) and (b) In a spreadsheet, we can calculate numerically:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t) \cdot dt}$$

Let us plot the given data:



This is quite similar to the RTD of a CSTR, so the reactor behaves as one CSTR.

(c) Mean residence time is calculated following the procedure explained in other problems, obtaining 32.97 (Run 1), 32.53 (Run 2), and 32.98 s (Run 3) (32.83 average value).

Volume of the reactor can be calculated:

$$\bar{t} = \frac{V}{Q} = t_m = \frac{V}{50} = 32.83 \,\mathrm{s}$$

resulting V = 1641.31

(d) Mass of tracer can be calculated by applying:

$$dN = Q_0 C(t) dt$$
$$N = Q_0 \int_0^\infty C(t) dt$$

The calculation gives N = 1382 mg (Run 1), N = 1412 mg (Run 2), and N =1480 mg (Run 3).

Problem 1.7 The following data correspond to a 22501 reactor that is fed 1501/s:

<i>t</i> (s)	0	2	4	6	8	10	12	14	16	18
p(t)	0.00	0.02	0.03	0.05	0.1	0.19	0.32	0.47	0.6	0.71

<i>t</i> (s)	20	22	24	26	28	30	32	34	36	38	40
p(t)	0.80	0.86	0.90	0.93	0.95	0.97	0.98	0.98	0.99	0.99	1.00

Estimate:

- (a) The Peclet number for the dispersion model.
- (b) The number of reactors for the model of stirred TIS.

Solution to Problem 1.7

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

The given function p(t) should correspond to F(t) data, i.e., to a step tracer run, as the value of this function is continuously growing from 0 to 1. These data have been plotted to verify that the trend is as expected. Before beginning to look for the solution that they ask us for, previous calculations must be made:

<i>t</i> (s)	$p_t(t)$	E(t)	E(t)∙dt	t·E(t)	Integral	$(t-t_m)^2 \cdot E(t)$	Integral
0	0	0	0.02	0		0	
2	0.02	0.01	0.01	0.02	0.02	1.994	1.994
4	0.03	0.005	0.02	0.02	0.04	0.734	2.728
6	0.05	0.01	0.05	0.06	0.08	1.024	1.759
8	0.1	0.025	0.09	0.2	0.26	1.648	2.673
10	0.19	0.045	0.13	0.45	0.65	1.685	3.334
12	0.32	0.065	0.15	0.78	1.23	1.103	2.789
14	0.47	0.075	0.13	1.05	1.83	0.337	1.440
16	0.6	0.065	0.11	1.04	2.09	0.001	0.338
18	0.71	0.055	0.09	0.99	2.03	0.194	0.195
20	0.8	0.045	0.06	0.9	1.89	0.677	0.872
22	0.86	0.03	0.04	0.66	1.56	1.037	1.715
24	0.9	0.02	0.03	0.48	1.14	1.242	2.279
26	0.93	0.015	0.02	0.39	0.87	1.464	2.706
28	0.95	0.01	0.02	0.28	0.67	1.411	2.876
30	0.97	0.01	0.01	0.3	0.58	1.927	3.338
32	0.98	0.005	0	0.16	0.46	1.261	3.187
34	0.98	0	0.01	0	0.16	0.000	1.261
36	0.99	0.005	0	0.18	0.18	1.976	1.976
38	0.99	0	0.01	0	0.18	0.000	1.976
40	1	0.005		0.2	0.2	2.851	2.851
		Sum =	1.00		16.12		42.29

The first thing to do is to calculate E(t) by using the data from F(t). This is done by numerical derivation, i.e.,

$$E(t) = \frac{\Delta F(t)}{\Delta t} = \frac{F^{t+1} - F^t}{\Delta t}$$

Once E(t) is known, both t_m and σ^2 (whose equations are shown in the header of the table) can be calculated.

When we already have the values of both t_m and σ^2 , we can calculate the required values.

The first model that is studied is the TIS. The parameter of such a model is n_t :

$$n_{\rm t} = \frac{t_m^2}{\sigma^2} = 6.14$$
 tanks

In order to be able to compare the E(t) obtained by the model with the E(t) obtained experimentally, it is also necessary to calculate $\overline{t} = 42.29/6.14 = 2.62$ s. On the other hand, to determine the deviation between the points obtained experimentally and with the method, the sum of the squared differences between all the points has been calculated:

Deviation =
$$\sum_{\text{all data}} (E(t)_{\text{calculated}} - E(t)_{\text{measured}})^2$$



Since the deviation is of the order of $2.36 \cdot 10^{-3}$, it can be concluded that the method can well predict the experimental E(t) values.

For the dispersion model, the first thing to calculate is the Bo number. In this case, the operation that has been done is: $\sigma^2 = 2Bo$, so Bo = 21.14.

Since Bo is greater than 0.01, a closed–closed system or an o–o system must be chosen. In this exercise, we will use the o–o assumption. The first thing that is done is to calculate the Bo with the equations that govern this o–o dispersion model:

$$t_m = \overline{t} \cdot (1 + 2 \cdot Bo)$$
$$\left(\frac{\sigma}{t_m}\right)^2 = 2 \cdot Bo + 8 \cdot Bo^2$$

Obtaining Bo = 0.074. The next step is to calculate E(t) with the closed-closed dispersion model. To do this, the following equation is used:





Problem 1.8 Consider a continuous reactor fed with a flow Q_0 with a composition C_{A0} . Both operating variables are held constant. The (total) volume of the reactor is V_R and the space time, τ , is defined based on this volume. The kinetics obeys the expression $(-r_A) = kC_A^a$, and there are no secondary reactions. The reactor is modeled as three identical continuous reactors, perfectly stirred, but it is considered that there is also a certain current "mixed" between the three cameras, which is equal to $\alpha \cdot Q_0$. To visualize this, analyze the following diagram:



Get the dynamic expressions for $\frac{dC_{A1}}{dt}$, $\frac{dC_{A2}}{dt}$ and $\frac{dC_{A3}}{dt}$ as functions of C_{A0} , C_{A1} , C_{A2} , C_{A3} , α , τ , a, and k, as required.

Solution to Problem 1.8

We will assume well-mixed behavior in all three reactors but consider the accumulation term in the mass balance. In this sense, in the first reactor:

Input + Generation = Output + Accumulation

$$n_{A,in} + r_A V = n_{A,out} + V \frac{dC_A}{dt}$$
$$Q_0 C_{A0} + \alpha Q_0 C_{A2} + \left(-kC_{A1}^a\right) V = (1+\alpha)Q_0 C_{A1} + V \frac{dC_{A1}}{dt}$$

Dividing by the flow rate Q_0 :

$$\begin{split} C_{A0} &+ \alpha C_{A2} \left(-k C_{A1}^{a} \right) \bar{t} = (1+\alpha) C_{A1} + \bar{t} \frac{\mathrm{d} C_{A1}}{\mathrm{d} t} \\ \frac{\mathrm{d} C_{A1}}{\mathrm{d} t} &= \frac{C_{A0} + \alpha C_{A2} - (1+\alpha) C_{A1}}{\bar{t}} - \left(k C_{A1}^{a} \right) \end{split}$$

In the second reactor:

$$\begin{aligned} (1+\alpha)Q_0C_{A1} + \alpha Q_0C_{A3} + \left(-kC_{A2}^a\right)V &= (1+\alpha)Q_0C_{A2} + \alpha Q_0C_{A2} + V\frac{\mathrm{d}C_{A2}}{\mathrm{d}t} \\ \frac{\mathrm{d}C_{A2}}{\mathrm{d}t} &= \frac{(1+\alpha)C_{A1} + \alpha C_{A3} - (1+2\alpha)C_{A2}}{\bar{t}} - kC_{A2}^a \end{aligned}$$

10

And in the third one:

$$(1+\alpha)Q_0C_{A2} + \left(-kC_{A3}^a\right)V = (1+\alpha)Q_0C_{A3} + V\frac{dC_{A3}}{dt}$$
$$\frac{dC_{A3}}{dt} = \frac{(1+\alpha)C_{A2} - (1+\alpha)C_{A3}}{\bar{t}} - kC_{A3}^a$$

Problem 1.9 Draw the E(t) curves for the following systems, with each system represented in a separate sketch:

- (a) An ideal PFR with a volume of 21 and a feed rate of 11/min.
- (b) An ideal CSTR with a volume of 21 and a feed rate of 11/min.
- (c) An ideal PFR with a volume of 21, followed by an ideal CSTR with a volume of 21. The feed flows in at a rate of 11/min.
- (d) An ideal CSTR with a volume of 21, followed by an ideal PFR with a volume of 21. The feed flows in at a rate of 11/min.
- (e) An ideal CSTR with a volume of 21 in parallel with an ideal PFR with a volume of 21. The feed, with a volume flow rate of 1 l/min, is evenly split between the two reactors: 0.5 l/min to the CSTR and 0.5 l/min to the PFR. After the reactors, the streams are mixed. Provide the E(t) curve for the entire system, not for each individual reactor.

Solution to Problem 1.9

 $t_{\rm PFR}$

(a) An ideal PFR (volume 21, feed 11/min):



(b) An ideal CSTR (volume 21, feed 11/min).



(c) An ideal PFR (volume 21) is followed by an ideal CSTR (volume 21). The feed has a volume flow rate of 1 l/min.

$$= \frac{2}{1} = 2 \min, \quad \overline{t_{\text{CSTR}}} = \frac{2}{1} = 2 \min$$

4 2

- (d) An ideal CSTR (volume 21) is followed by an ideal PFR (volume 21). The feed has a volume flow rate of 1 l/min.Same *E*(*t*) as in case (c).
- (e) An ideal CSTR (volume 21) in parallel with an ideal PFR (volume 21). The feed (volume flow rate 1 l/min) is equally divided over the reactors: 0.5 l/min to the CSTR and 0.5 l/min to the PFR. After the two reactors, the streams are mixed together. Give the E(t) curve of the complete system, not of each individual reactor.

$$\overline{t_{\text{PFR}}} = \frac{2}{0.5} = 4 \text{ min}, \quad \overline{t_{\text{CSTR}}} = \frac{2}{0.5} = 4 \text{ min}$$

$$E(t) \quad \text{Area (PFR)} = 0.5$$

$$Area (\text{CSTR}) = 0.5$$

$$4 \quad t \text{ (min)}$$

Problem 1.10 During the "Chemical Reactor Engineering" course, there was a problem that involved sketching the E(t) curve for a system of interconnected ideal reactors. Several answers were provided, and four of the sketches are as follows:



Answer (1) appears to be the correct answer.

- (a) Sketch a possible system of interconnected ideal reactors, resulting in sketch 1.
- (b) What systems of interconnected reactors correspond to the other sketches?
- (c) Sketch the corresponding *F*-curve for each system.
 - Denote PFRs in your answer as $P_1, P_2 \dots$ and CSTRs as $T_1, T_2 \dots$, with respective volumes $V_{P1}, V_{P2}, \dots, V_{T1}, V_{T2}, \dots$ Denote the various volume flow rates as $Q_1, Q_2 \dots$
- (d) Sketch the figure yourself, and put relevant information in it (points of intersection, areas, etc.), expressed in V_{P1}, V_{P2}, ..., V_{T1}, V_{T2}, ..., Q₁, Q₂, ...

If the first-order irreversible reaction $A \rightarrow$ products, with rate constant *k*, takes place in this system of reactors, what is the conversion at the outlet of the system? (again, expressed in $V_{P1}, V_{P2}, ..., V_{T1}, V_{T2}, ..., Q_1, Q_2, ...)$?

Solution to Problem 1.10

(a) and (b)





(e) In the PFR:

$$C_{\rm A1} = C_{\rm A0} \cdot \exp(-k\overline{t_{\rm PFR}}) = C_{\rm A0} \cdot \exp\left(-\frac{kV_{\rm PFR}}{Q_0 - Q_b}\right)$$

Then, in the CSTR:

$$C_{\mathrm{A2}} = \frac{C_{\mathrm{A1}}}{1 + k \cdot \overline{t_{\mathrm{CSTR}}}} = \frac{C_{\mathrm{A0}} \cdot \exp\left(-\frac{kV_{\mathrm{PFR}}}{Q_0 - Q_b}\right)}{1 + k \cdot \frac{V_{\mathrm{CSTR}}}{Q_0 - Q_b}}$$

In the mix point, at the end of the system:

$$\begin{aligned} Q_0 C_{\text{Aout}} &= (Q_0 - Q_b) \cdot C_{\text{A2}} + Q_b \cdot C_{\text{A0}} \\ C_{\text{Aout}} &= \frac{(Q_0 - Q_b)}{Q_0} \cdot \frac{C_{\text{A0}} \cdot \exp\left(-\frac{kV_{\text{PFR}}}{Q_0 - Q_b}\right)}{1 + k \cdot \frac{V_{\text{CSTR}}}{Q_0 - Q_b}} + \frac{Q_b}{Q_0} \cdot C_{\text{A0}} \end{aligned}$$

Problem 1.11 At time t = 0, a step change in tracer concentration occurs in the feed of a reactor with unknown flow behavior. At the reactor outlet, the following *F*-curve is measured:



- (a) Please sketch the *E*-curve of this unknown reactor, including all relevant information in the sketch.
- (b) Which combination of ideal reactors has the same *E*-curve as the unknown reactor?
- (c) What is the residence time of the unknown reactor?
- (d) If the reaction $A \rightarrow B$, with a rate $(-r_B) = -4C_A \text{ kmol/m}^3 \cdot \text{min}$, occurs in the unknown reactor at the residence time determined in part (c), what will be the conversion of A?

Solution to Problem 1.11

(a)





(c) Residence time is: $t = 0.33 \cdot 0 + 0.66 \cdot 0.5 = 0.33$ min

(d) $A \rightarrow B$, with $(-r_B) = -4C_A \text{ kmol/m}^3 \cdot \text{min}$, takes place in the unknown reactor. What will be the conversion of A? In a PFR, first-order reaction: $X_A = 1 - \exp(-k\overline{t})$

$$X_{\rm A} = 1 - \exp(-4 \cdot 0.33) = 0.732$$

As only 66% of the flow passes through the reactor, the correct conversion is:

$$X_{\text{Afinal}} = 0.732 \cdot 0.66 = 0.483$$

Problem 1.12 Three ideal PFRs with volumes of 2, 4, and 6 m^3 are interconnected, as shown in the figure below. The water feed, with a volume flow rate (Q_0) of 3 m^3 /min, is divided between the parallel PFRs as indicated:



(a) At t = 0, a pulse of salt is injected into the feed at point A. Please sketch the salt concentration versus time curves at points B, C, D, and E. Make sure to indicate the scale divisions on the axes.After conducting the experiment described above, the split ratio of the feed over

the two PFRs is changed such that in the new situation $Q_1 = 1 \text{ m}^3/\text{min}$ and $Q_2 = 1 \text{ m}^3/\text{min}$. Once again, at t = 0, a pulse of 2 mol of salt is injected into the feed at point A.

- (b) Sketch the salt concentration versus time curves at points B, C, D, and E, considering the new split ratio. Indicate the scale divisions on the axes.
- (c) Sketch the *F*-curve for the overall system in both situations. Please note that the volume of the tubing connecting the PFRs can be neglected.

(b)



(c) In the first situation:



And in the second:



Problem 1.13 During the oxidation of phenol to cyclohexanone, assume that the reaction rate is given by $r = k \cdot C_A$ ("A" being phenol) when excess O₂ is present. The following parameter values are known:

V = 66 ml	$Q_0 = 3 \text{ ml/min}$	$C_{\rm A0} = 0.1 {\rm mol/l}$
$C_{\rm A}$ (out of the reactor) = 0.01 mol/l	$T = 80 \degree \text{C}$	P = 3 MPa

- (a) What is the residence time for this reactor? Solve the steady-state PFR material balance. Given the steady-state outlet concentration of A, what is the value of the rate constant *k*?
- (b) To perform an RTD step test on the reactor, two inert solvents are used: toluene and cyclohexane. The reactor (PFR) begins with toluene flowing through at steady state. At time t = 0, a valve is turned introducing the cyclohexane flow and cutting off the toluene flow. The measured RTD is shown in the figure. What is the mean residence time for the reactor?



(c) From the data, estimate the dimensionless dispersion number, Bo, describing this reactor.

Solution to Problem 1.13:

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) Residence time is: $t = V/Q_0 = 66/3 = 22$ min For the PFR in steady state: $dn_A = r_A dV$, which for a first-order reaction gives:

 $C_{\rm A} = C_{\rm A0} \cdot \exp(-k\bar{t})$

In the present case:

 $0.01 = 0.1 \cdot \exp(-k \cdot 22)$

Giving a value of $k = 0.1 \text{ min}^{-1}$

Time (s)	F(t)	<i>E(t)</i> (s ⁻¹)	$E(t) \cdot \Delta t$	t·E(t)	t·E(t)·∆t	$(t-t_m)^2 \cdot E(t)$	$(t-t_m)^2 \cdot E(t) \cdot \Delta t$
1200	0	0.0010	0.05	1.20	61.25	101	5062.5
1250	0.05	0.0010	0.05	1.25	161.25	1	62.5
1300	0.1	0.0040	0.2	5.20	231.25	605	30 2 50
1350	0.3	0.0030	0.15	4.05	223.75	1654	82687.5
1400	0.45	0.0035	0.35	4.90	395.00	8409	840 875
1500	0.8	0.0020	0.1	3.00	113.75	6503	325125
1550	0.9	0.0010	0.05	1.55	58.75	4651	232 562.5
1600	0.95	0.0005	0.05	0.80	40.00	6301	630125
1700	1	0.0006					
		Sum=	1	t_m (s)=	1245	σ^2 (s ²)	2146750
				t_m (min)=	20.75	σ^2 (min ²)	596.32

(b) We can read in the plot the time-F(t) data and do the corresponding calculations:

The value of E(t) is calculated by using a numerical method for deriving the F(t) values read in the graph. In this way:

$$E^t = \frac{F^{t-1} - F^t}{\Delta t}$$

The value of t_m is calculated by integrating (i.e. sum) of the values of $(t \cdot E(t) \cdot \Delta t)$. As we can see, in this system $\overline{t} \neq t_m$. In fact, $\overline{t} > t_m$, so we would expect to get the E(t) signal later. This is probably due to the fact that flow rate is not measured correctly, or that there is a dead volume not contributing to the total residence time in the reactor. In any case, we first try to find the Bo number for applying the dispersion model. Assuming that Bo < 0.01, we can do $\sigma^2 = 2 \cdot Bo$, and we find that Bo $\gg 0.01$, so the assumption is not correct. For Bo > 0.01 and assuming o–o conditions:

$$\left(\frac{\sigma}{t_m}\right)^2 = 2 \cdot \mathrm{Bo} + 8 \cdot \mathrm{Bo}^2$$

finding that Bo = 0.3113 that is actually quite a high value (Bo > 0.2). We can assume that the reactor would be similar to a CSTR. Indeed, if we apply the TIS model, we find that:

$$n_{\rm t} = \frac{t_m^2}{\sigma^2} = \frac{20.75^2}{596.32} = 0.72$$
 tanks





Do a mass balance in this system for a tracer pulse input and determine the residence time distribution function in the case where tank 1 is very small compared to tank 2 and the transfer speed between the reactors is very small.

Solution to Problem 1.14

If we propose a molar balance on the tracer, with a pulse injected at t = 0 for each of the tanks, we obtain:

Accumulation = Input – Output (there is no tracer generation)

$$V_1 \frac{dC_{T1}}{dt} = Q_1 C_{T2} - (Q_0 C_{T1} + Q_1 C_{T1}) \quad \text{(in the first tank)}$$
$$V_2 \frac{dC_{T2}}{dt} = Q_1 C_{T1} - Q_1 C_{T2} \quad \text{(in the second tank)}$$

where C_{T1} and C_{T2} are, respectively, tracer concentrations in both reactors. These two differential equations are coupled and should be solved simultaneously.

In this model, the two adjustable parameters are the flow rate exchanged (Q_1) and the volume of the most agitated region (V_1) . Remember that the measured volume (V) is the sum of V_1 and V_2 . We will call β the fraction of the total flow that is transferred between both reactors:

$$Q_1 = \beta \cdot Q_0$$

and α to the fraction of the total volume that corresponds to the most agitated area:

$$V_1 = \alpha \cdot V \rightarrow V_2 = (1 - \alpha) \cdot V$$

On the other hand, the average time (\bar{t}) is given by the quotient V/Q_0 . The initial conditions (t = 0) for this model are: (i) $C_{T1} = (C_{T1})_0$, and (ii) $(C_{T2})_0 = 0$. Analytical solution is possible in the present case and is the following:

$$\left[\frac{C_{\text{T1}}}{(C_{\text{T1}})_0}\right]_{\text{pulse}} = \frac{(\alpha m_1 + \beta + 1)\exp\left(\frac{m_2 t}{\overline{t}}\right) - (\alpha m_2 + \beta + 1)\exp\left(\frac{m_1 t}{\overline{t}}\right)}{\alpha (m_1 - m_2)}$$

being:

$$m_1, m_2 = \left[\frac{1-\alpha+\beta}{2\alpha(1-\alpha)}\right] \left[-1 \pm \sqrt{1 - \frac{4\alpha\beta(1-\alpha)}{(1-\alpha+\beta)^2}}\right]$$

Previous equation shows that, if tank 1 is small compared to 2 (α small), and the transfer speed between both reactors is small (β small), the second exponential term tends to 1 during the first part of the response to an impulse injection. During the second part, the first exponential term tends to 0. If we represent the logarithm of the tracer concentration versus time, the response curve will tend to a straight line at both ends of the curve, and the parameters will be obtained from the slopes (m_1 for $t \to \infty$ and m_2 for $t \to 0$) and the cut points of both lines (for $t \to \infty$, the cut point is $-\{\alpha m_2 + \beta + 1\}/\alpha\{m_1 - m_2\}$).

Problem 1.15 Figure shows a combination of ideal reactors used to model a real reactor.



- (a) Qualitatively sketch the RTD (i.e. E(t), F(t)) that would result if two of the following combinations of ideal reactors were connected in series (i.e. n = 1).
- (b) How would your results change if two were connected in series (i.e. n = 2)?
- (c) How about n = 5 or 10?

Solution to Problem 1.15

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

For n = 1, we have a signal corresponding to one CSTR with interchange displaced by a value of time corresponding to the RFP residence time. If n = 2, the signal is displaced two times:



For values of "*n*" higher, the system would behave as a PFR, with residence time *n* times the residence time of the first reactor.

In Problem 3.2, we will see that the transfer function of this system of reactors is (n = 1):

$$E(s) = \frac{(\exp(-\overline{t_1}s)) \cdot \left(\frac{1}{1+\overline{t_2}s}\right)}{1+\beta-\beta \left(\frac{1}{1+\overline{t_3}s}\right)\left(\frac{1}{1+\overline{t_2}s}\right)}$$

being β the ratio Q_1/Q_0 . For a system where n = 2:

$$E(s) = \left[\frac{(\exp(-\overline{t_1}s)) \cdot \left(\frac{1}{1+\overline{t_2}s}\right)}{1+\beta-\beta\left(\frac{1}{1+\overline{t_3}s}\right)\left(\frac{1}{1+\overline{t_2}s}\right)}\right]^2$$

The inverse of the Laplace transform is a very complicated function E(t).

We can do a simulation using Matlab[®]. For a system consisting of two CSTRs with flow rate Q_1 between them, expression for the pulse run concentration is that shown in the previous problem, but now α is the ratio $V_2/(V_2 + V_3)$.

For example, for n = 1-4, with $V_1 = 0.9$ V and $Q_1 = 0.1 \cdot Q_0$, $\overline{t_{\text{RFP}}} = 10$ and $\overline{t_{\text{CSTR}}} = 20$, we can do:

```
clear all
close all
alfa=0.9;
beta=0.9;
tm pfr=10;
tm cstrs=20;
m 1=[(1-alfa+beta)/(2*alfa*(1-alfa))]*[-1+((1-(4*alfa*beta*(1-alfa))/
    (1-alfa+beta)^2))^0.5];
m 2=[(1-alfa+beta)/(2*alfa*(1-alfa))]*[-1-((1-(4*alfa*beta*(1-alfa))/
    (1-alfa+beta)^2))^0.5];
t=0:150;
td=(t-tm pfr)/tm cstrs;
E1=((alfa*m 1+beta+1)*exp(m 2*td)-(alfa*m 2+beta+1)*exp(m 1*td))/
    alfa/(m_1-m_2);
E1=(t>tm_pfr).*E1;
subplot(2,2,1), plot(t,E1)
area=sum(E1*1);
E1=E1/area;
tmdistrib=sum(E1.*t*1)
title('n=1')
xlabel('Time')
ylabel('E(t)')
응응응응
```

```
E2=conv(E1,E1);
t2=2*t(1):2*t(end);
area=sum(E2*1);
E2=E2/area;
tmdistrib=sum(E2.*t2*1)
subplot(2,2,2), plot(t2,E2)
title('n=2')
xlabel('Time')
ylabel('E(t)')
***
E3=conv(E2,E1);
t3=3*t(1):3*t(end);
area=sum(E3*1);
E3=E3/area;
tmdistrib=sum(E3.*t3*1)
subplot(2,2,3), plot(t3,E3)
title('n=3')
xlabel('Time')
ylabel('E(t)')
응응응응
E4=conv(E3,E1);
t4=4*t(1):4*t(end);
area=sum(E4*1);
E4=E4/area;
tmdistrib=sum(E4.*t4*1)
subplot(2,2,4), plot(t4,E4)
title('n=4')
xlabel('Time')
ylabel('E(t)')
```

Getting:





During the calculation, we can check that, for n = 1, $t_m = \overline{t_{\text{PFR}}} + \overline{t_{\text{CSTR}}} = 30$. For n = 2, $t_m = 2 \cdot (\overline{t_{\text{PFR}}} + \overline{t_{\text{CSTR}}}) = 60$ For n = 3, $t_m = 3 \cdot (\overline{t_{\text{PFR}}} + \overline{t_{\text{CSTR}}}) = 90$ For n = 4, $t_m = (\overline{t_{\text{PFR}}} + \overline{t_{\text{CSTR}}}) = 120$ And comparing all four distributions:



Problem 1.16 A tracer step input experiment is being performed, feeding pure water, switching to salt water, and analyzing the conductivity at the outlet. The data represented in the figure was obtained.

- (a) What will the output signal be like if the tracer had been injected into pulse?
- (b) Calculate the mean residence time of the reactor.



Solution to Problem 1.16

(a) What we have obtained is a cumulative RTD (i.e. F(t) curve), and it is easy to find the time that the tracer will exit with C_{max} :



Mean residence time:

$$t_m = \int_0^\infty t \cdot E(t) dt = \int_{0.3}^{t_F} t \cdot 0.87 dt = \frac{0.87}{2} (1.45^2 - 0.3^2) = 0.8754 \text{ min}$$

The E(t) function is:



We can check that:

$$\int_0^\infty E(t) dt = \int_{0.3}^{1.45} 0.87 dt = 0.87(1.45 - 0.3) = 1$$

Problem 1.17 A test is performed with a tracer pulse, and a curve is obtained that follows the expression $C = (t - 2)^2$ for $0 \le t \le 2$ and C = 0 at any other time. Calculate the mean residence time using the equation for E(t) and F(t).

Solution to Problem 1.17

In the reactor, we have a pulse that input gives:

$$C(t) = (t-2)^2$$



The area under the curve is defined between 0 and 2 (time where C(t) equals to zero). And in this way:

$$\int_0^\infty C(t) \mathrm{d}t = \int_0^2 (t-2)^2 \mathrm{d}t = 2.6667$$

And so:

$$E(t) = \frac{(t-2)^2}{2.6667}$$

Following the definition of F(t):

$$F(t) = \int_0^t E(t) dt = \int_0^t \frac{(t-2)^2}{2.6667} dt = 0.124\,984t^3 - 0.749\,906t^2 + 1.499\,81t + K$$

being "K" an integration constant. By definition, we know that:

$$\lim_{t \to \infty} F(t) = 1 = \lim_{t \to 2} F(t)$$

so the constant "K" should be equal to zero.

Problem 1.18 A reaction system is described by the following model:



At a given moment, the system presents values of $\alpha = 0.1$ and $\beta = 0.9$. A series of reforms are carried out in the system, and it is achieved that $\alpha = 0.9$ and $\beta = 0.1$.

- (a) Qualitatively draw the response of the system to a tracer impulse, comparing the two situations.
- (b) Also, draw the corresponding F(t) curves for both situations.
- (c) Indicate what reforms had to be made to achieve this change.

Solution to Problem 1.18

(a) In this system, the residence time compared to that expected is:

$$\overline{t_{\text{actual}}} = \frac{V_m}{Q_{\text{reactor}}} = \frac{\alpha V}{(1-\beta)Q} = \frac{\alpha}{(1-\beta)}\overline{t_{\text{expected}}}$$

As we have that $\alpha = 0.1$ and $\beta = 0.9$ at the beginning:

$$\overline{t_{\text{actual}}} = \frac{0.1}{(1-0.9)}\overline{t_{\text{expected}}} = \overline{t_{\text{expected}}}$$

In the second case:

$$\overline{t_{\text{actual}}} = \frac{0.9}{(1-0.1)}\overline{t_{\text{expected}}} = \overline{t_{\text{expected}}}$$

So it will be very difficult to observe these changes. Nevertheless, the bypass produces a very important peak at time equal to zero in both situations, but the amount of tracer passing through the bypass is much higher in the first case. We can have something similar to:



(b) The cumulative time function would have the following aspect:



(c) Usually, a better agitation is procured to eliminate dead volumes. Also, reduction of bypass flow is achieved with better agitation or by changing the reactor filling.

Problem 1.19 In a tracer input experiment, a perfect pulse is injected, and the following distribution is obtained:

- (a) Calculate the mean residence time of the reactor.
- (b) What will the output signal be like if the tracer has been injected in step?



Solution to Problem 1.19

(a) In the signal obtained, the total area is 1.0.5 + (0.5.2/2) = 1 (just checking).



The straight-line connecting points (0, 1) and (0.5, 3) is E(t) = 1 + 4t, so:

$$t_m = \int_0^\infty t \cdot E(t) dt = \int_0^{0.5} t \cdot (1+4t) dt = 0.2917 \min$$

(b) If a step tracer run is done, we will get:



Problem 1.20 A commercial-scale distillation tray is being studied for residence time using a fiber optic technique. A pulse of a 10 g/l solution of Rhodamine-B dye was injected into the downcomer of the top tray. The response data, summarizing the time (min) and corresponding output voltage (V), are provided as follows:

Time (min)	Output voltage (V)
0.0	0.00
0.1	0.00
0.2	2.80
0.3	4.48

Time (min)	Output voltage (V)
0.4	3.32
0.5	1.70
0.6	0.84
0.7	0.39
0.8	0.18
0.9	0.11
1.0	0.07
1.1	0.03
1.2	0.04
1.3	0.01
1.4	0.01
1.5	0.01
1.6	0.00
1.7	0.01
1.8	0.00
1.9	0.00

Note: The output voltage is proportional to the concentration of the dye.

- (a) Determine the mean residence time and the characteristic F(t) curve for this system.
- (b) Use the dispersion model and the variance method to determine Bo (Bodenstein number) and Pe (Peclet number).
- (c) Estimate the number of equal-sized CSTRs in series that would exhibit a comparable dispersion to the observed experimental data.
- (d) Provide comments on the obtained results.

Solution to Problem 1.20

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) Using similar techniques to those mentioned in other problems, we easily find:

C(t)	C(t)·∆t	E(t)	$E(t) \cdot \Delta t$	F(t)	t∙E(t)	t·E(t)·∆t	$(t-t_m)^2 \cdot E(t)$	$(t-t_m)^2$ $E(t)\cdot\Delta t$
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.140	0.000	0.100	0.000	0.000	0.000	0.000	0.000
2.800	0.364	2.000	0.260	0.200	0.400	0.020	0.064	0.003
4.480	0.390	3.200	0.279	0.520	0.960	0.068	0.020	0.004
3.320	0.251	2.371	0.179	0.757	0.949	0.095	0.001	0.001
1.700	0.127	1.214	0.091	0.879	0.607	0.078	0.018	0.001

46	1	Non-ideal Flow and Reactor Characterization
----	---	---

C(t)	C(t)·∆t	E(t)	E(t)·∆t	F(t)	t∙E(t)	t∙E(t)∙∆t	$\frac{(t-t_m)^2}{E(t)}$	$\frac{(t-t_m)^2}{E(t)\cdot\Delta t}$
0.840	0.062	0.600	0.044	0.939	0.360	0.048	0.029	0.002
0.390	0.029	0.279	0.020	0.966	0.195	0.028	0.029	0.003
0.180	0.015	0.129	0.010	0.979	0.103	0.015	0.023	0.003
0.110	0.009	0.079	0.006	0.987	0.071	0.009	0.021	0.002
0.070	0.005	0.050	0.004	0.992	0.050	0.006	0.019	0.002
0.030	0.004	0.021	0.003	0.994	0.024	0.004	0.011	0.002
0.040	0.003	0.029	0.002	0.997	0.034	0.003	0.019	0.002
0.010	0.001	0.007	0.001	0.998	0.009	0.002	0.006	0.001
0.010	0.001	0.007	0.001	0.999	0.010	0.001	0.007	0.001
0.010	0.001	0.007	0.000	0.999	0.011	0.001	0.009	0.001
0.000	0.000	0.000	0.000	0.999	0.000	0.001	0.000	0.000
0.010	0.001	0.007	0.000	1.000	0.012	0.001	0.012	0.001
0.000	0.000	0.000	0.000	1.000	0.000	0.001	0.000	0.001
0.000		0.000		1.000	0.000	0.000	0.000	0.000
$\Sigma(C(t)dt) =$	= 1.4	$\Sigma(E(t)dt) =$	= 1.0		<i>t_m</i> =	= 0.38 min	σ^2	$= 0.029 \min^{2}$



(b) For the dispersion model to be applied, first we should assume Bo < 0.01 and then:

$$\sigma^2 = 2 \cdot Bo$$

We obtain Bo = 0.014, so this assumption is almost valid. We can do now:

$$Pe = \frac{1}{Bo} = 69.05$$

(c) With the values of t_m and σ^2 , using the TIS model:

$$n_{\rm t} = \frac{t_m^2}{\sigma^2} = \frac{0.38^2}{0.029} = 4.98 \text{ tanks} \approx 5 \text{ tanks}$$

(d) This reactor has a very small dispersion, and so the number of tanks that should be used in the TIS model is quite high. The system is completely solvable and its RTD is:

$$E = \frac{1}{\overline{t} \cdot \sqrt{4 \cdot \pi \cdot \text{Bo}}} \cdot \exp\left[-\frac{\left(1 - \frac{t}{\overline{t}}\right)^2}{4 \cdot \text{Bo}}\right]$$

We can compare the experimental and estimated E(t) curves using the spread-sheet:





can be described by the time dependence of the effluent concentration of the species as follows:

$$C_{\rm A} = 0$$
 for $0 < t < 8.5$ min
 $C_{\rm A} = 10^5 \,{\rm e}^{-2t}$ for $t > 8.5$ min

for C_A in pmol/ml. The curve is generated by injecting a pulse of a sample containing species A into a solvent flowing through the chromatographic column at a constant flow rate.

- (a) Determine the mathematical form of the F(t) curve corresponding to the response of the pulse test.
- (b) Use the *F*(*t*) curve to calculate the average residence time of species A in the column.

Solution to Problem 1.21

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) The total area of tracer is:

$$\int_0^\infty C(t) dt = \int_0^\infty 10^5 \cdot \exp(-2t) dt = 2.01 \cdot 10^{-3}$$

So, for *t* > 8.5:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t) dt} = 4.83 \cdot 10^7 \cdot \exp(-2t)$$

We can check that:

$$\int_{0}^{\infty} E(t) \mathrm{d}t = 1$$

In this way:

$$F(t) = \int_0^t E(t) dt = \int_0^t (4.83 \cdot 10^7 \cdot \exp(-2t)) dt = 1 - 2.415 \cdot 10^7 \exp(-2t)$$

(b)

$$t_m = \int_0^\infty t \cdot E(t) dt = \int_{8.5}^\infty t \cdot (4.83 \cdot 10^7 \cdot \exp(-2t)) dt = 8.89 \min(-2t) + 10^{-10} + 10^{$$

We can use a numerical method too. In the spreadsheet corresponding to this problem, values of time are given and C_A is calculated. Following the procedure shown before in other problems:

$$\Sigma(C(t)dt) = 0.001 \ 204 \ 66$$
$$\Sigma(E(t)dt) = 1.0$$
$$t_m = 9.29 \ \text{min}$$
$$\sigma^2 = 0.229 \ \text{min}^2$$



Doing the graphical plot:

Problem 1.22 The techniques discussed in this chapter for analyzing residence time distribution functions can be applied to study flow conditions in streams or rivers, particularly when assessing the dispersion of pollutants from a source. The following data was obtained from a study of the South Platte River. The average flow rate is 15.68 m^3 /s, the length of the reach is 6065 m, and the natural concentration of K⁺ ions in the stream is 8.2 mg/l.

At time zero, 453.5 kg of K_2CO_3 was dumped into the upstream end of the reach. Samples were periodically collected at the downstream end of the reach and analyzed for K⁺ ions. The results are presented in the table below.

t (min)	K ⁺ at downstream (g/m	³)
0.0	8.2	
60.0	8.2	
75.0	8.2	
90.0	8.2	
105.0	8.4	
120.0	9.6	
130.0	13.6	

t (min)	K ⁺ at downstream (g/m ³)
132.5	14.8
134.0	14.8
138.0	14.6
142.5	13.2
150.0	12.8
165.0	10
180.0	9.2
195.0	8.2
210.0	8.2
300.0	8.2

(a) Calculate the fraction of the tracer (K_2CO_3) that was recovered.

(b) Based on the recovered amount of tracer, calculate the F(t) curve. Additionally, compute the average residence time and plot the effluent concentration of K⁺ ions exceeding the background level.

Solution to Problem 1.22

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

(a) Subtracting the natural K⁺ level, we find:

t (min)	C(t)	C(t)·∆t	E(t)	E(t)·∆t	F(t)	t·E(t)·∆t	$(t-t_m)^2 \cdot E(t) \cdot \Delta t$
0.0	0	0.00	0.000	0.000	0.000	0.000	0.000
60.0	0	0.00	0.000	0.000	0.000	0.000	0.000
75.0	0	0.00	0.000	0.000	0.000	0.000	0.000
90.0	0	1.50	0.000	0.006	0.000	0.000	0.000
105.0	0.2	12.00	0.001	0.051	0.013	0.666	9.368
120.0	1.4	34.00	0.006	0.144	0.101	5.992	33.747
130.0	5.4	15.00	0.023	0.063	0.330	18.389	36.857
132.5	6.6	9.90	0.028	0.042	0.399	8.331	9.322
134.0	6.6	26.00	0.028	0.110	0.441	5.577	4.366
138.0	6.4	25.65	0.027	0.108	0.550	14.945	6.567
142.5	5.0	36.00	0.021	0.152	0.645	15.178	1.840
150.0	4.6	48.00	0.019	0.203	0.791	22.234	3.212
165.0	1.8	21.00	0.008	0.089	0.905	31.294	32.824
180.0	1	7.50	0.004	0.032	0.968	15.124	68.928
195.0	0	0.00	0.000	0.000	0.968	5.707	42.389
210.0	0	0.00	0.000	0.000	0.968	0.000	0.000
300.0	0		0.000		0.968	0.000	0.000

$$\Sigma(C(t)dt) = 236.55$$
$$\Sigma(E(t)dt) = 1.0$$
$$t_m = 143.44 \text{ min}$$
$$\sigma^2 = 249.42 \text{ min}^2$$

We can see that:

$$\sum (C(t)\mathrm{d}t) = 236.55 \,\frac{\mathrm{g}\cdot\min}{\mathrm{m}^3}$$

Taking into account that the flow rate is $15.68 \text{ m}^3/\text{s}$, we have that the amount recovered is:

$$M = 236.55 \,\mathrm{g} \cdot \frac{\mathrm{min}}{\mathrm{m}^3} \cdot 15.68 \,\frac{\mathrm{m}^3}{\mathrm{s}} \cdot 60 \,\frac{\mathrm{s}}{\mathrm{min}} = 222\,546.24 \,\mathrm{g} = 222.5 \,\mathrm{kg}$$

This means that only 49% of the K⁺ dumped is recovered.

(b)



Problem 1.23 By injecting brine into an experimental continuous reactor, a signal is obtained at the exit given by:

t (min)	1	3	5	7	9	11	13
<i>C</i> (g/l)	0	2	3	4	2	1	0

The flow rate at the inlet is 101/min.

- (a) How much salt was injected?
- (b) Calculate E(t), F(t), mean residence time, and variance.

Solution to Problem 1.23

For details refer the Wiley website at http://www.wiley-vch.de/ISBN9783527354115

To solve this problem, we should use a spreadsheet. First, data given in the statement is introduced, and then we should do the following calculations:

t (min)	C(t)	$C(t) \cdot \Delta t$	E(t)	F(t)	t·E(t)·∆t	$\frac{(t-t_m)^2}{E(t)}$	$\frac{(t-t_m)^2}{E(t)\cdot\Delta t}$
1	0.00	0.00	0.0000	0.0000	0	0	0
3	2.00	4.00	0.0833	0.1667	0.5000	1.0208	2.0417
5	3.00	6.00	0.1250	0.4167	1.2500	0.2813	0.5625
7	4.00	8.00	0.1667	0.7500	2.3333	0.0417	0.0833
9	2.00	4.00	0.0833	0.9167	1.5000	0.5208	1.0417
11	1.00	2.00	0.0417	1.0000	0.9167	0.8438	1.6875
13	0.00	0.00	0.0000	1.0000	0.0000	0.0000	0.0000
$\Sigma(C(t)\mathrm{d}t) = 24.00$				$t_m = 6.50 \min$			$\sigma^2 = 5.42 \min^2$

The total area of the C(t) curve is:

Area =
$$\int_0^\infty C(t) dt = \sum_{\text{all points}} C(t) \Delta t = 24 \frac{g}{l} \cdot \min$$

The total amount of tracer introduced is:

$$M_0 = Q_0 \int_0^\infty C(t) dt = 10 \frac{1}{\min} \cdot 24 \frac{g \cdot \min}{l} = 240 g$$

For calculating the RTD:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t) \cdot dt} = \frac{C(t)}{24}$$

And:

$$t_m = \int_0^\infty t \cdot E(t) dt = \sum_{\text{all points}} t \cdot E(t) \cdot \Delta t = 6.5 \text{ min}$$

In a similar way, variance is calculated:

$$\sigma^{2} = \sum_{\text{all points}} (t - t_{m})^{2} \cdot E(t) \cdot \Delta t = 5.41 \text{ min}^{2}$$

Finally, we can calculate F(t) by attending to its definition:

$$F(t) = \sum_{\text{all points at time} < t} E(t) \cdot \Delta t$$



We can check the form of the graphs showing the distributions: