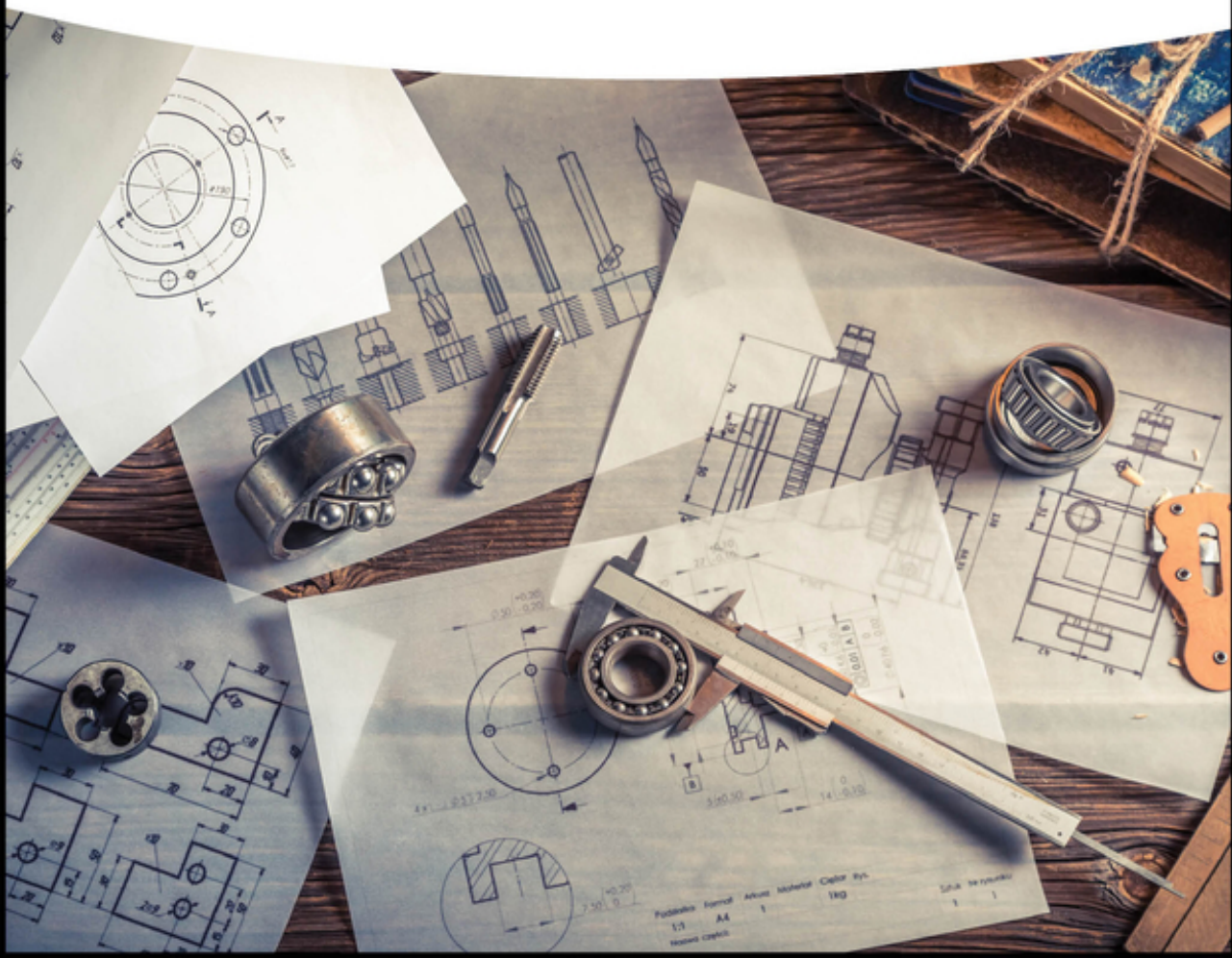


Juan A. Conesa

Problem Solving in Chemical Reactor Design



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To my beloved wife, Marga, and children, Margarita, Juan, Pablo, and Miguel.

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Preface

This book has been written after more than two decades of teaching experience in chemical reactor engineering. During these years, I have been collecting problems posed to undergraduate and master's students, which are now compiled here along with their solutions. This is not a basic chemical reactor engineering (CRE) book; instead, it covers the design of nonideal, catalytic, multiphase, and biochemical reactors.

Following the publication of my book *Chemical Reactor Design: Mathematical Modeling and Applications* in 2019, this book addresses aspects not covered in basic textbooks dedicated to reactor design. The concepts introduced in my earlier book are further developed here through solved examples. This approach aims to help the reader gain a deeper understanding of reactor design procedures, especially in the context of nonideal and heterogeneous reactors.

This collection of solved problems in advanced chemical reactor engineering provides in-depth coverage of complex reactor design issues, such as the design of catalytic or biochemical reactors. It is not a basic book covering simple concepts.

The book is accompanied by electronic materials, including spreadsheets and Matlab® programs, which can be downloaded from the Wiley website at <http://www.wiley-vch.de/ISBN9783527354115>.

The tools used in this book are not complex, and the solutions are presented in a simplified manner. I primarily use spreadsheets and occasionally incorporate Matlab. Importantly, the programs are designed to be highly understandable.

Elche (Spain)
May 2024

Juan A. Conesa

Nomenclature

Suggested units are indicated for each variable.

$A_{m \times n}$	matrix of convolution
C	concentration (usually mol/m ³ , or kg/m ³)
C_{As}	concentration of A in the surface (mol/m ³)
c_p	calorific capacity of the reacting flow (J/K · g)
C_p	concentration of product “P” (mol/m ³)
C_T	total concentration (mol/m ³)
d_p	particle diameter (m)
D	dilution rate (s ⁻¹)
D_A	diffusion coefficient of species A (m ² /s)
D_{AB}	diffusion coefficient (diffusivity) of A in B (m ² /s)
D_e	effective diffusion coefficient (m ² /s)
E	(in the reaction rates context) → activation energy (J/mol)
E	(in the RTD context) → residence time distribution function, RTD (—)
F	integral form of the residence time distribution function (—)
g_A	generation term of a mole balance (mol/s)
h	heat transfer coefficient (J/K · s)
$H(s)$	transfer function (—) (Laplace space)
$h(t)$	time-dependent transfer function (—)
k	kinetic constant (units depend on the kinetic law)
k_0	pre-exponential factor of the kinetic constant (units depend on the reaction order)
k_L	mass transfer coefficient in the liquid phase (mol/s · m ² /(mol/m ³) = m/s)
K_M	Michaelis constant (g/l)
K_S	Monod constant (g/l)
L	characteristic length (m)
$L\{h(t)\}$	Laplace transform of function $h(t)$
M	tracer mass (g or mol)
N	amount of substance (mol)
n_A	molar flow of component “A” (mol/s or mol/s · m ²)
N_{ad}	dimensionless adiabatic temperature increase (—)
N_c	dimensionless cooling capacity (—)
n_t	number of tanks in the tanks-in-series model (—)

n_T	total molar flow (mol/s)
q	heat flux (J/s)
Q	volumetric flowrate (m ³ /s)
q_C	heat flux in cooling media (J/s)
R	radius (m)
r_A'''	reaction (or process) rate based on the volume of catalyst particles (mol/s · m ³)
r_A''	reaction (or process) rate based on the volume of reacting species (mol/s · m ³)
r_A'	reaction (or process) rate based on the weight of catalyst (mol/s · g)
r_A	reaction (or process) rate based on the external catalyst surface (mol/s · m ²)
R_g	universal gas constant (J/mol · K)
s	(in the Laplace transform context) → main variable in the Laplace space
S	section (m ²)
T	temperature (K)
t	time (s)
\bar{t}	average residence time (= V/Q) (s)
T_C	temperature of the cooling media (K)
t_m	first moment of the RTD; mean value of time (s)
U	global heat transfer coefficient (J/K · s)
u	linear velocity (m/s)
V	volume (m ³)
V_d	dead volume (m ³)
V_p	volume with plug flow regime (m ³)
W	weight of catalyst (g)
We	Weisz modulus (—)
$X(s)$	stimulus function (—) (Laplace space)
$x(t)$	time-dependent stimulus function (—)
X_A	molar conversion of reactant A (—)
$Y(s)$	response to stimulus function (—) (Laplace space)
$y(t)$	time-dependent response to stimulus function (—)

Greek Symbols

τ	tortuosity factor (—)
α	fraction of volume of a subsystem (—)
β	fraction of flow passing through a subsystem (—)
δ	dirac delta function (—)
μ	growth rate per unit of cell (1/s)
ϵ_s	solid load (m ³ solid/m ³ reactor)
ϵ_G	gas fraction (m ³ gas/m ³ reactor)
ϵ_L	liquid fraction (m ³ liquid/m ³ reactor)
ϵ_b	bed porosity (m ³ void/m ³ reactor)
σ^2	variance (s ²)
σ	standard deviation (s)

η effectiveness (—)
 ΔH_r enthalpy of a reaction (kJ/mol)

Subscripts

i actual position
 $i + 1$ position of the following interval
 $i - 1$ position of the preceding interval
 S surface
 0 inlet conditions
 F fluid
 C catalyst
 R reactor

Superscripts

t actual time
 $t + 1$ time of the following interval
 $t - 1$ time of the previous interval

Part I

Non-ideal Flow Characterization and Chemical Reaction

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:

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

In a step tracer run:

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

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):

$$\sigma^2 = \int_0^{\infty} (t - t_m)^2 \cdot E(t) dt$$

The square root of the variance, σ , is called standard deviation.

Average residence time:

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

RTD in Ideal Reactors

For the plug flow reactor (PFR):

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

For the continuous stirred tank reactor (CSTR):

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

Tanks-in-series (TIS) Model

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

$$\sigma^2 = \frac{t_m^2}{n_t}$$

$$n_t = \frac{t_m^2}{\sigma^2}$$

Dispersion Model

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

Bo < 0.01

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

$$t_m = \bar{t} = \frac{V}{Q}$$

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

Bo > 0.01, Closed-Closed Recipient

$E(t)$ is only integrable by numerical methods.

$$\bar{t} = t_m$$

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

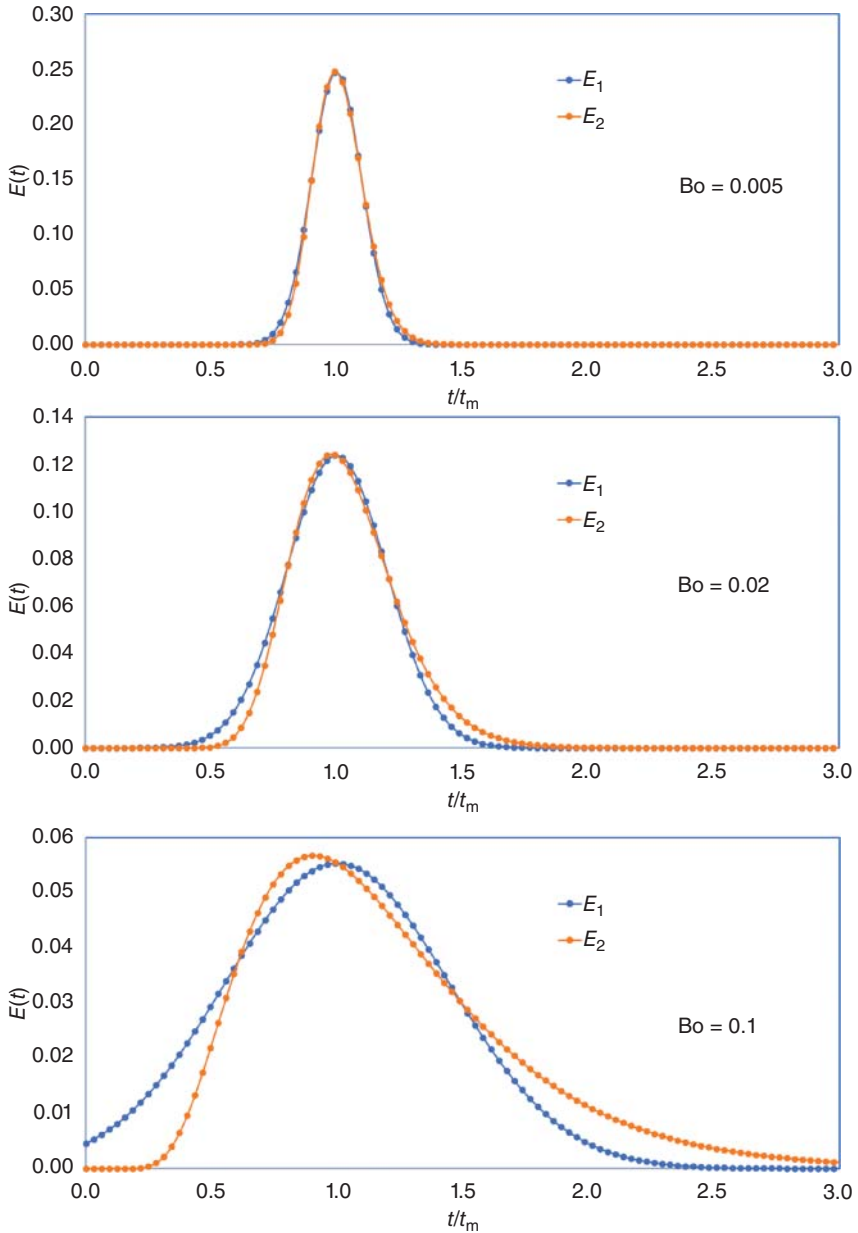
Bo > 0.01, Open-Open Recipient

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

$$t_m = \bar{t} \cdot (1 + 2 \cdot Bo)$$

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

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 (KMnO_4) 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 KMnO_4 .

- 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 $I(t)$.
- 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>

(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:

t (s)	$C(t)$	$C(t)\Delta t$	$E(t)$	$t \cdot E(t)$	$t \cdot E(t) \cdot \Delta t$	$\frac{(t - t_m)^2}{E(t)}$	$\frac{(t - t_m)^2}{E(t) \cdot \Delta t}$	$F(t)$	$I(t)$
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		
$\Sigma(C(t)\Delta t) = 771$			$t_m = 10.98$ s			$\sigma^2 = 46.88$ s ²			

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:

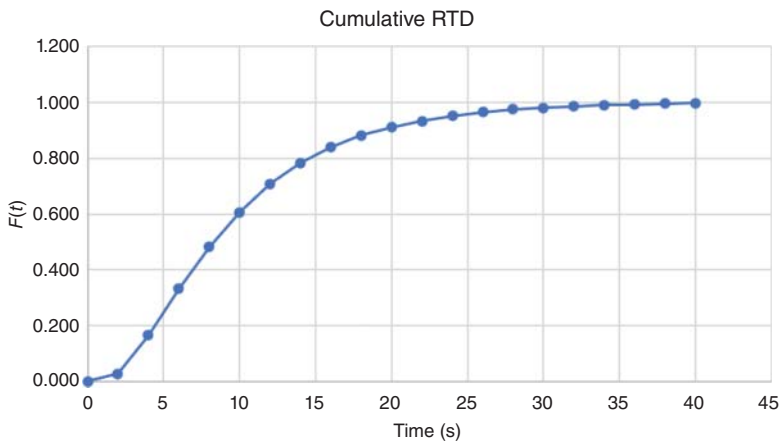
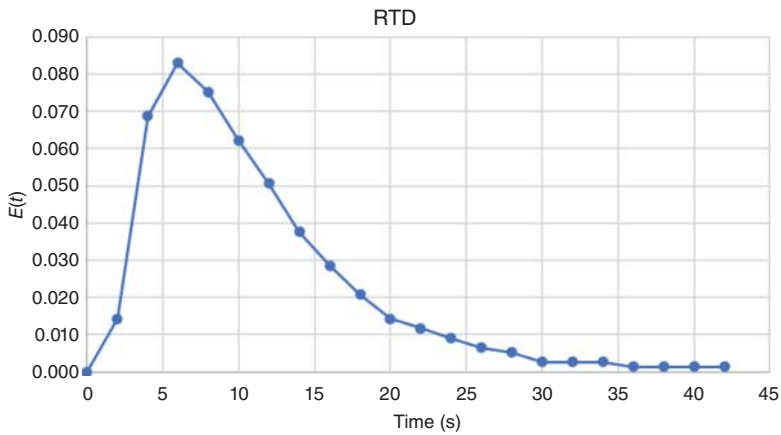
$$\sigma^2 = \sum_{\text{all points}} (t - t_m)^2 \cdot E(t) \cdot \Delta t = 46.88 \text{ s}^2$$

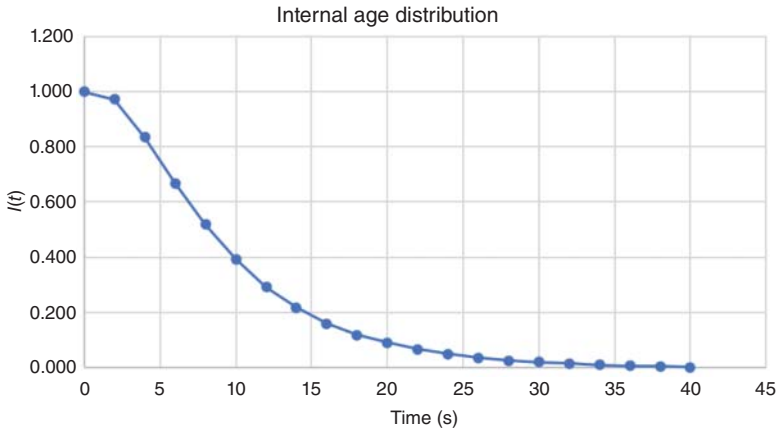
Finally, we can calculate $F(t)$ and $I(t)$ according to their definitions:

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

$$I(t) = 1 - F(t)$$

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:

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

We obtain $Bo = 11.24 \gg 0.01$, so this assumption is not valid.

Assuming now $Bo > 0.01$ and closed-closed recipient:

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

From that:

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

and we obtain $Bo = 0.2413$, and $Pe = 1/Bo = 4.14$.

On the other hand, if an o-o recipient is assumed:

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

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

- Calculate the RTD of this reactor.
- What fraction of the fluid spends more than 3 minutes in the reactor? Make a plot of the procedure.
- 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>

- 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}	$I(t)$	$F(t)$	$E(t) = \Delta F/\Delta t$
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	

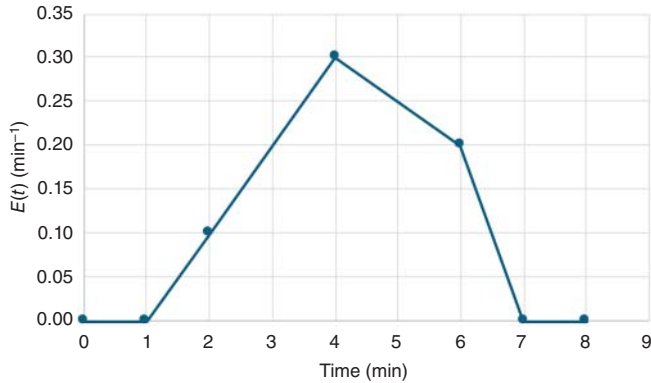
In the table, $I(t)$ is derived directly from the data, and:

$$F(t) = 1 - I(t)$$

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

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

Obtaining:



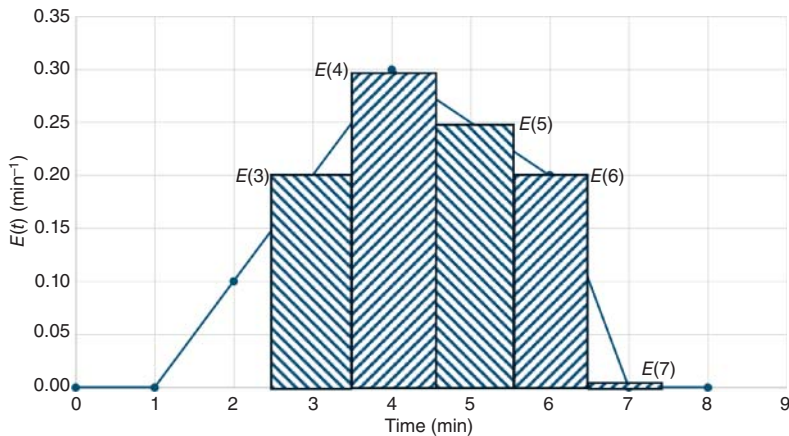
- (b) For calculating the fraction of fluid that spends a time in the reactor, we use the definition of $E(t)$:

$$\text{Fluid passing more than 3 minutes} = f_{>3} = \int_3^{\infty} E(t)dt$$

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:

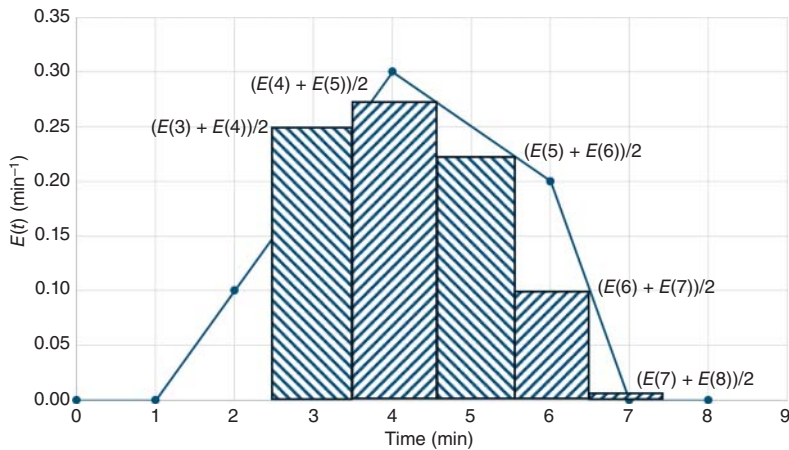


Obviously, this is a rough approximation. A better approximation would involve using smaller time increments, but this is not possible with the obtained data.

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

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

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:

t (min)	$c \times 10^5$ (g/l)	t (min)	$c \times 10^5$ (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