Web17.4 The Tanks-in-Series (T-I-S) One-Parameter Model

$n = ?$

In this section we discuss the use of the tanks-in-series (T-I-S) model to describe nonideal reactors and calculate conversion. The T-I-S model is a one-parameter model. We will analyze the RTD to determine the number of ideal tanks, *n*, in series that will give approximately the same RTD as the nonideal reactor. Next, we will apply the chemical reaction engineering algorithm developed in Chapters 1 through 5 to calculate conversion. We are first going to develop the RTD equation for three tanks in series (Figure W17-1) and then generalize to *n* reactors in series to derive an equation that gives the number of tanks in series that best fits the RTD data.

Web17.4.1 Developing the *E*-Curve for the T-I-S Model

The RTD will be analyzed from a tracer pulse injected into the first reactor of three equally sized CSTRs in series. The trace concentration, $C_3(t)$ is measured at the exit of the third reactors.

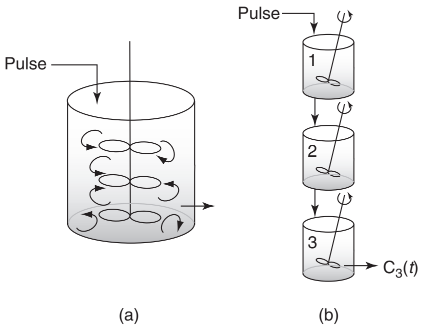


Figure W17-1 Tanks in series: (a) real system; (b) model system.

Using the definition of the RTD presented in Section 16.2, the fraction of material leaving the system of three reactors (i.e., leaving the third reactor) that has been in the system between time *t* and $t + \Delta t$ is

$$E(t)\,\Delta t = \frac{vC_3(t)\,\Delta t}{N_0} = \frac{C_3(t)}{\int_0^\infty C_3(t)\,dt}\,\Delta t$$

In Figure 2-9, we saw how tanks in series could approximate a PFR.

Then

$$E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)\,dt} \qquad \text{(W17-1)}$$

In this expression, $C_3(t)$ is the concentration of tracer in the effluent from the third reactor and the other terms are as defined previously.

By carrying out mass balances on the tracer sequentially for reactors 1, 2, and 3, it is shown on the CRE Web site in the *Expanded Material* for Chapter 18 that the exit tracer concentration for reactor 3 is

$$C_3 = \frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i} \tag{W17-2}$$

where $\tau_i = \tau_1 = \tau_2 = \tau_3 = \tau/n = \frac{V}{v_0 n}$ and V is the volume of the real system and v_0 is the flow rate through the reactors,

Substituting Equation (W17-2) into Equation (W17-1), we find that

$n = 3$

$$E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)dt} = \frac{C_0 t^2/(2\tau_i^2)e^{-t/\tau_i}}{\int_0^\infty \frac{C_0 t^2 e^{-t/\tau_i}}{2\tau_i^2}dt}$$

$$= \frac{t^2}{2\tau_i^3} e^{-t/\tau_i} \tag{W17-3}$$

Generalizing this method to a series of n CSTRs gives the RTD for n CSTRs in series, $E(t)$:

RTD for equal-size tanks in series

$$\boxed{E(t) = \frac{t^{n-1}}{(n-1)!\tau_i^n} e^{-t/\tau_i}} \tag{W17-4}$$

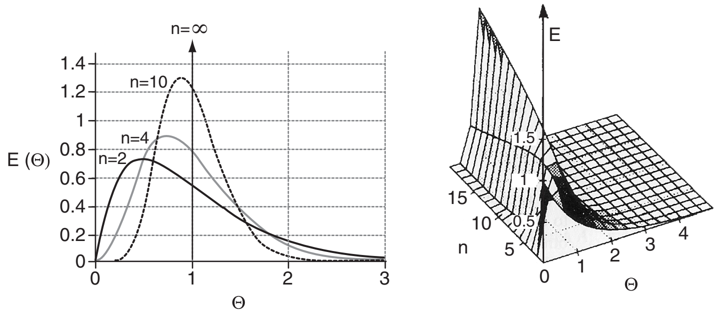
We can make Equation (W17-4) a bit more useful if we put in the dimensionless form in terms of $E(\Theta)$. Because the total reactor volume is nV_i, then $\tau_i = \tau/n$, where τ represents the total reactor volume divided by the flow rate, v , we have

$$E(\Theta) = \tau E(t) = \frac{n(n\Theta)^{n-1}}{(n-1)!} e^{-n\Theta} \tag{W17-5}$$

where $\Theta = t/\tau$ = Number of reactor volumes of fluid that have passed through the reactor after time t.

Here, $(E(\Theta)\, d\Theta)$ is the fraction of material exiting between dimensionless time Θ and time $(\Theta + d\Theta)$.

Figure 17-2 illustrates the RTDs of various numbers of CSTRs in series in a two-dimensional plot (a) and in a three-dimensional plot (b). As the number becomes very large, the behavior of the system approaches that of a plug-flow reactor.



(a) (b)

Figure W17-2 Tanks-in-series response to a pulse tracer input for different numbers of tanks.

We can determine the number of tanks in series by calculating the dimensionless variance σ_Θ^2 from a tracer experiment.

$$\sigma_\Theta^2 = \frac{\sigma^2}{\tau^2} = \int_0^\infty (\Theta - 1)^2 E(\Theta)\, d\Theta \tag{W17-6}$$

$$= \int_0^\infty \Theta^2 E(\Theta)\, d\Theta - 2\int_0^\infty \Theta E(\Theta)\, d\Theta + \int_0^\infty E(\Theta)\, d\Theta \tag{W17-7}$$

$$\boxed{\sigma_\Theta^2 = \int_0^\infty \Theta^2 E(\Theta)\, d\Theta - 1} \tag{W17-8}$$

$$= \int_0^\infty \Theta^2 \frac{n(n\Theta)^{n-1}}{(n-1)!} e^{-n\Theta}\, d\Theta - 1$$

$$\sigma_\Theta^2 = \frac{n^n}{(n-1)!}\int_0^\infty \Theta^{n+1} e^{-n\Theta}\, d\Theta - 1 \tag{W17-9}$$

$$= \frac{n^n}{(n-1)!}\left[\frac{(n+1)!}{n^{n+2}}\right] - 1$$

As the number of tanks increases, the variance decreases.

$$\sigma_\Theta^2 = \frac{1}{n} \tag{W17-10}$$

The number of tanks in series is calculated by calculating the mean, τ, and the variance, σ^2, from the experimentally determined RTD curve

$$\boxed{n = \frac{1}{\sigma_\Theta^2} = \frac{\tau^2}{\sigma^2}} \tag{W17-11}$$

This expression represents the number of tanks necessary to model the real reactor as n ideal tanks in series. If the number of reactors, n, turns out to be small, the reactor characteristics turn out to be those of a single CSTR or perhaps two CSTRs in series. At the other extreme, when *n* turns out to be large, we recall from Chapter 2 that the reactor characteristics approach those of a PFR.

Web17.4.2 Calculating Conversion for the T-I-S Model

If the reaction is first order, we can use Equation (5-15) to calculate the conversion

$$X = 1 - \frac{1}{(1 + \tau_i k)^n} \tag{5-15}$$

where

$$\tau_i = \frac{V}{v_0 n}$$

It is acceptable (and usual) for the value of *n* calculated from Equation (W17-11) to be a noninteger in Equation (5-15) to calculate the conversion. For reactions other than first order, an integer number of reactors must be used and sequential mole balances on each reactor must be carried out. If, for example, $n = 2.53$, then one could calculate the conversion for two tanks and also for three tanks to bound the conversion. The conversion and effluent concentrations would be solved sequentially using the algorithm developed in Chapter 5; that is, after solving for the effluent from the first tank, it would be used as the input to the second tank as shown below (*http://www.umich.edu/~elements/5e/18chap/expanded_ch18_TISmodel.pdf*).

TABLE W17-1 TANKS-IN-SERIES SECOND-ORDER REACTION

<table>
<tr><th>Two-Reactor System</th><th>Three-Reactor System</th></tr>
<tr><td>For two equally sized reactors
$$V = V_1 + V_2$$
$$V_1 = V_2 = \frac{V}{2}$$
$$\tau_2 = \frac{V_2}{v_0} = \frac{V/2}{v_0} = \frac{\tau}{2}$$</td><td>For three equally sized reactors
$$V = V_1 + V_2 + V_3$$
$$V_1 = V_2 = V_3 = V/3$$
$$\tau_1 = \tau_2 = \tau_3 = \frac{V/3}{v_0} = \frac{\tau}{3}$$</td></tr>
<tr><td colspan="2">For a second-order reaction, the combined mole balance, rate law, and stoichiometry for the first reactor gives
$$\tau = \frac{C_{\mathrm{Ain}} - C_{\mathrm{Aout}}}{k_1 C_{\mathrm{Aout}}^2}$$
Solving for C_{Aout}
$$C_{\mathrm{Aout}} = \frac{-1 + \sqrt{1 + 4k\tau C_{\mathrm{Ain}}}}{2k\tau}$$</td></tr>
</table>

TABLE W17-1 TANKS-IN-SERIES SECOND-ORDER REACTION (*Continued*)

Two-Reactor System: $\tau_2 = \dfrac{\tau}{2}$ Three-Reactor System: $\tau_3 = \dfrac{\tau}{3}$

Solving for the exit concentration from reactor 1 for each reactor system gives

$$C_{A1} = \frac{-1+\sqrt{1+4\tau_2 k C_{A0}}}{2\tau_2 k} \qquad C'_{A1} = \frac{-1+\sqrt{1+4\tau_3 k C_{A0}}}{2\tau_3 k}$$

The exit concentration from the second reactor for each reactor system gives

$$C_{A2} = \frac{-1+\sqrt{1+4\tau_2 k C_{A1}}}{2\tau_2 k} \qquad C'_{A2} = \frac{-1+\sqrt{1+4\tau_3 k C'_{A1}}}{2\tau_3 k}$$

Balancing on the third reactor for the three-reactor system and solving for its outlet concentration, C'_{A3}, gives

$$C'_{A3} = \frac{-1+\sqrt{1+4\tau_3 k C'_{A2}}}{2\tau_3 k}$$

The corresponding conversions for the two- and three-reactor systems are

$$X_2 = \frac{C_{A0} - C_{A2}}{C_{A0}} \qquad X'_3 = \frac{C_{A0} - C'_{A3}}{C_{A0}}$$

For $n = 2.53$, $(X_2 < X < X'_3)$

Web17.4.3 Tanks-in-Series versus Segregation for a First-Order Reaction

We have already stated that the segregation and maximum mixedness models are equivalent for a first-order reaction. The proof of this statement was left as an exercise in Problem P17-3$_B$. We can extend this equivalency for a first-order reaction to the tanks-in-series (T-I-S) model

$$\boxed{X_{\text{T-I-S}} = X_{\text{seg}} = X_{\text{mm}}} \tag{W17-12}$$

The proof of Equation (W17-12) is given in the below, in Web Example 17-1.

See Table W17-2 where A = 2.5 for Tanks-In-Series to calculate the boundary conversion when the number of tanks is $n = 2$ and $n = 3$.

Web Example 17–1 Equivalency of Models for a First-Order Reaction

Show that $X_{\text{T–I–S}} = X_{\text{MM}}$ for a first-order reaction

$$A \xrightarrow{k} B$$

Solution

For a first-order reaction, we already showed in Problem P17-3$_B$ that

$$\boxed{X_{\text{Seg}} = X_{\text{MM}}}$$

Therefore, we only need to show $X_{\text{Seg}} = X_{\text{T-I-S}}$.
For a first-order reaction in a batch reactor the conversion is

$$X = 1 - e^{-kt} \tag{WE17-1.1}$$

Segregation Model

$$\bar{X} = \int_0^\infty X(t)E(t)dt = \int_0^\infty (1 - e^{-kt})E(t)dt \tag{WE17-1.2}$$

$$= 1 - \int_0^\infty e^{-kt}E(t)dt \tag{WE17-1.3}$$

Using Maclaurin's series expansion gives

$$e^{-kt} = 1 - kt + \frac{k^2t^2}{2} + \text{Error} \tag{WE17-1.4}$$

Neglecting the error term

$$\bar{X} = 1 - \int_0^\infty \left[1 - kt + \frac{k^2t^2}{2}\right]E(t)dt \tag{WE17-1.5}$$

$$\bar{X} = \tau k - \frac{k^2}{2}\int_0^\infty t^2E(t)dt \tag{WE17-1.6}$$

To evaluate the second term, we first recall Equation (16-23) for the variance

$$\sigma^2 = \int_0^\infty (t-\tau)^2E(t)dt = \int_0^\infty t^2E(t)dt - 2\tau\int_0^\infty tE(t)dt + \tau^2\int_0^\infty E(t)dt \tag{WE17-1.7}$$

$$\sigma^2 = \int_0^\infty t^2E(t)dt - 2\tau^2 + \tau^2 \tag{WE17-1.8}$$

Rearranging Equation (WE17-1.8)

$$\int_0^\infty t^2E(t)dt = \sigma^2 + \tau^2 \tag{WE17-1.9}$$

Combining Equations (WE17-1.6) and (WE17-1.9), we find the mean conversion for the segregation model for a first-order reaction is

$$\boxed{\bar{X} = \tau k - \frac{k^2}{2}(\sigma^2 + \tau^2)} \tag{WE17-1.10}$$

Tanks in Series

Recall from Chapter 4, for *n* tanks in series for a first-order reaction, the conversion is

$$X = 1 - \frac{1}{\left(1 + \frac{\tau}{n}k\right)^n} \tag{WE17-1.11}$$

Rearranging yields

$$X = 1 - \left(1 + \frac{\tau}{n}k\right)^{-n} \tag{WE17-1.12}$$

We now expand in a binomial series

$$X = 1 - \left[1 - n\frac{\tau}{n}k + \frac{n(n+1)}{2}\frac{\tau^2 k^2}{n^2} + \text{Error}\right] \tag{WE17-1.13}$$

$$= k\tau - \frac{\tau^2 k^2}{2} - \frac{\tau^2 k^2}{2n} + \text{Error} \tag{WE17-1.14}$$

Neglecting the error gives

$$X = k\tau - \frac{k^2}{2}\left[\tau^2 + \frac{\tau^2}{n}\right] \tag{WE17-1.15}$$

Rearranging Equation (W17-12) in the form

$$\frac{\tau^2}{n} = \sigma^2 \tag{W17-12}$$

and substituting in Equation (WE17-1.15), the mean conversion for the T-I-S model is

$$\boxed{X = \tau k - \frac{k^2}{2}(\tau^2 + \sigma^2)} \tag{WE17-1.16}$$

We see that Equations (WE17-1.10) and (WE17-1.16) are identical; thus, the conversions are identical, and for a first-order reaction we have

Important result

$$\boxed{X_{\text{T-I-S}} = X_{\text{Seg}} = X_{\text{MM}}} \tag{WE17-1.17}$$

But this is true only for a first-order reaction.

Analysis: For first-order reactions, we have shown that no matter how the molecules mix (macromixing, micromixing, T-I-S), the conversions predicted for each model are identical.