A First Course on Kinetics and Reaction Engineering

Activity 11.2b

The data in the table below were generated using the CSTRImpulseResponse simulator. Prior to the stimulus, the volume percent of tracer in the reactor feed was equal to 0%. The stimulus was an impulse containing 75 mL of tracer, the reactor volume was 10 L, and the feed rate was 10 L min^{-1}.

Time (min)	Concentration (g/L)
0	0
0.02	0.7238
0.15	0.6398
0.23	0.5808
0.35	0.5426
0.4	0.5039
0.52	0.4297
0.58	0.4222
0.75	0.3433
0.82	0.3187
1.02	0.2713
1.2	0.2361
1.47	0.1543
1.75	0.1327
1.9	0.1167
2.25	0.094
2.49	0.0466
2.99	0.0312

The stimulus was an impulse, so the age function, $F(\lambda)$, can be computed from the response using equation (1). Here, however, the response was measured as volume percent, not weight fraction. Assuming there is no volume change due to mixing, the two quantities are related according to equation (2), the mass flow rate is related to the known volumetric flow rate according to equation (3) and the mass of tracer is related to the volume of tracer according to equation (4). Upon substitution of equations (2) through (4) into equation (1), equation (5) results. Further noting that $V_{\%,0}$ = 0 and t_0 = 0 leads to equation (6), which can be used to calculate a value of $F(\lambda)$ for λ equal to each of the times at which the response was measured. Since $V_{\%,out}(t)$ takes the form of the data in the table above, and not an analytical function, the integration must be performed numerically, e. g. using the trapezoid rule (See Example 11.4). The resulting data can be plotted, as shown in Figure 1.

$$F\left(\lambda = t' - t_0\right) = \frac{\dot{M}\int_{t_0}^{t'}\left(w_{out}\left(t\right) - w_0\right)dt}{m_{tot}} \tag{1}$$

$$w_i = \frac{m_i}{m_{fluid}} = \frac{\rho_{tracer}}{\rho_{fluid}}\frac{\frac{m_i}{\rho_{tracer}}}{\frac{m_{fluid}}{\rho_{fluid}}} = \frac{\rho_{tracer}}{\rho_{fluid}}\frac{V_i}{V_{fluid}} = \frac{\rho_{tracer}}{\rho_{fluid}}\frac{V_{\%}}{100\%} \tag{2}$$

$$\dot{M} = \dot{V}\rho_{fluid} \tag{3}$$

$$m_{tot} = V_{impulse}\rho_{tracer} \tag{4}$$

$$F\left(\lambda = t' - t_0\right) = \frac{\dot{V}\int_{t_0}^{t'}\left(V_{\%,out}\left(t\right) - V_{\%,0}\right)dt}{\left(100\%\right)V_{impulse}} \tag{5}$$

$$F\left(\lambda = t'\right) = \frac{\dot{V}}{\left(100\%\right)V_{impulse}}\int_{t_0}^{t'}V_{\%,out}\left(t\right)dt \tag{6}$$

If the tested reactor obeys the assumptions for ideal CSTR, the age function should be given by equation (7). The average residence time, $\overline{t}$, that appears in equation (7) is found using equation (8). Substitution of equation (8) into equation (7) leads to equation (9) for the age function of an ideal CSTR that corresponds to the tested reactor. That age function is also plotted in Figure 1.

$$F_{CSTR}\left(\lambda\right) = 1 - \exp\left\{\frac{-\lambda}{\overline{t}}\right\} \tag{7}$$

$$\overline{t} = \frac{V}{\dot{V}} = \frac{10\text{ L}}{10\text{ L min}^{-1}} = 1.0\text{ min} \tag{8}$$

$$F_{CSTR}\left(\lambda\right) = 1 - \exp\left\{-\lambda\text{ min}^{-1}\right\} \tag{9}$$

The figure shows that within the experimental noise in the data, the measured age function values agree with the values predicted using the ideal CSTR model. As long as this reactor is not used to study extremely fast reactions, it is safe to model it as an ideal CSTR.

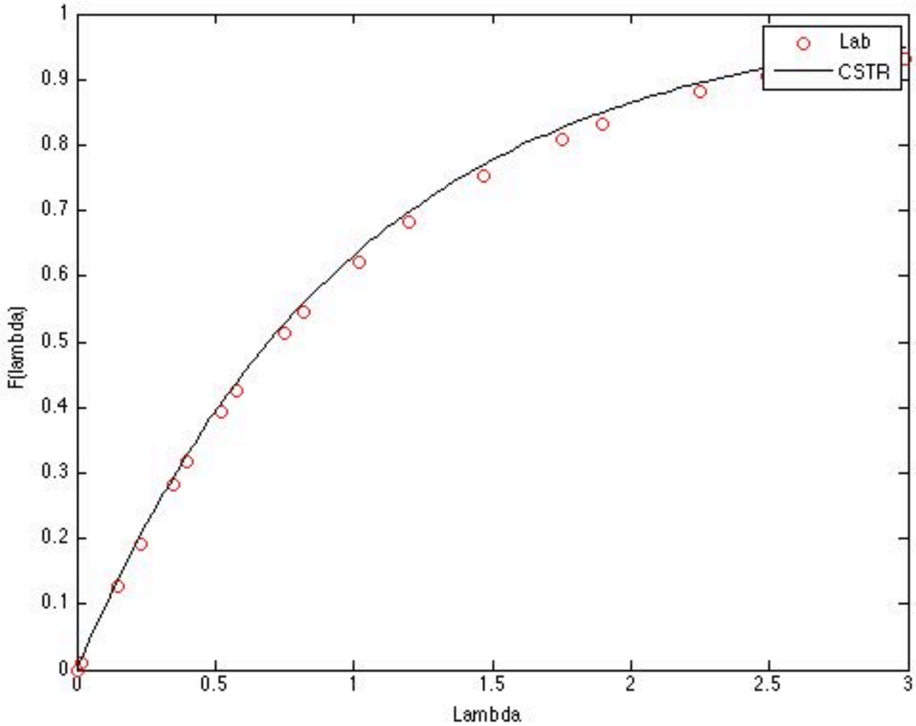

Figure 1. Comparison of the experimental and ideal age functions.

Important Note

If the flow rate was set to a high value, or if significant time was allowed to pass prior to the first sampling of the response, *it may appear that the reactor is not ideal*. The reason for this is related to the nature of the CSTR response in combination with the use of numerical integration of equation (6). When the impulse is first injected into the reactor, the concentration of tracer immediately jumps to its highest value and then begins to decay. If the first sampling of the response is delayed, then the first measured tracer concentration will be much smaller than the maximum value, and as a consequence, the numerical integral will be smaller than it should be. One tell-tale indicator of this problem will be that the age function will level off at a value less than 1.0. To illustrate, I repeated the analysis above, but deleted the second and third rows from the data table, simulating a situation where the first sampling was too late. The resulting age function plots are shown in Figure 2.

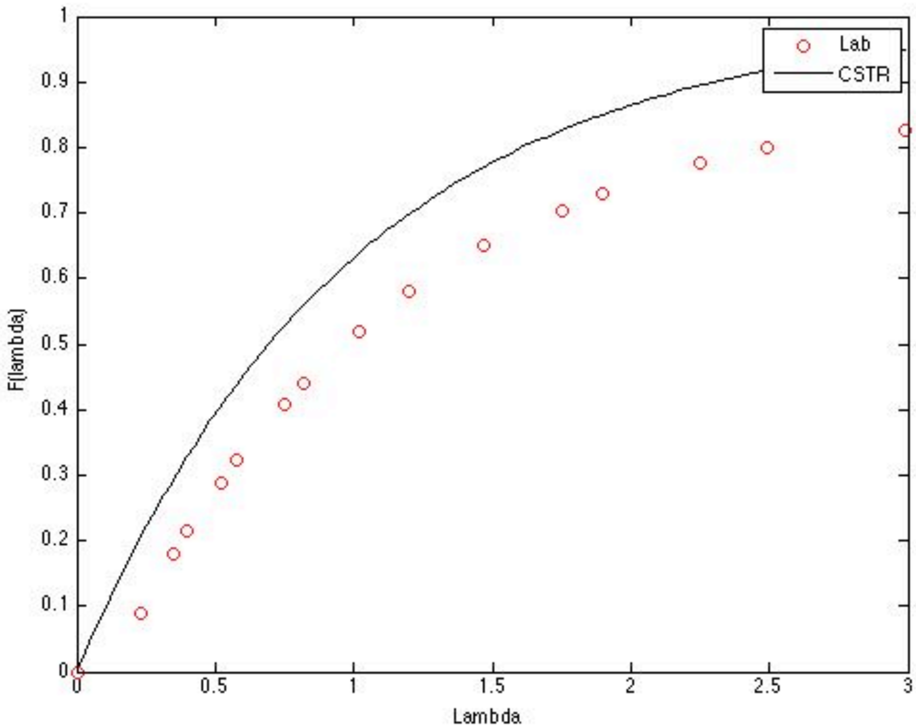

Figure 2. Comparison of the experimental and ideal age function when the first two measured responses are omitted.