

## A First Course on Kinetics and Reaction Engineering

### Activity 11.2a

The data in the table below were generated using the CSTRStepResponse simulator. Prior to the stimulus, the volume percent of tracer in the reactor feed was equal to 0%, and after the step change it was equal to 0.99%. The reactor volume was 10 L, and after the stimulus the feed rate was 20.2 L min<sup>-1</sup>.

<i>Time (min)</i>	<i>Outlet Tracer Volume Percent</i>
0	0
0.02	0.0565
0.05	0.0844
0.12	0.1971
0.15	0.2415
0.18	0.3209
0.23	0.3777
0.28	0.4505
0.35	0.4818
0.4	0.5488
0.48	0.6381
0.55	0.6544
0.63	0.7224
0.72	0.7613
0.8	0.777
0.88	0.8446
1	0.8349
1.08	0.8897
1.18	0.8999
1.32	0.9379
1.45	0.9283
1.59	0.9677
1.82	0.9453
1.99	0.9721
2.1	0.961
2.25	0.972
2.49	0.9649

The stimulus was a step change, 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). Upon substitution of equation (2) into equation (1) for each of the weight fractions and simplification, equation (3) results. Further noting that  $V_{\%,0} = 0$ ,  $t_0 = 0$  and  $V_{\%,f} = 0.99$  leads to equation (4), which can be used to calculate a value of  $F(\lambda)$  for  $\lambda$  equal to each of the times at which the response was measured. The resulting data can be plotted, as shown in Figure 1.

$$F(\lambda = t - t_0) = \frac{w_t - w_0}{w_f - w_0} \quad (1)$$

$$w_i = \frac{m_i}{m_{fluid}} = \frac{\rho_i}{\rho_{fluid}} \frac{\frac{m_i}{\rho_i}}{\frac{m_{fluid}}{\rho_{fluid}}} = \frac{\rho_i}{\rho_{fluid}} \frac{V_i}{V_{fluid}} = \frac{\rho_i}{\rho_{fluid}} \frac{V_{\%}}{100\%} \quad (2)$$

$$F(\lambda = t - t_0) = \frac{V_{\%,t} - V_{\%,0}}{V_{\%,f} - V_{\%,0}} \quad (3)$$

$$F(\lambda = t) = \frac{V_{\%,t}}{0.99\%} \quad (4)$$

If the tested reactor obeys the assumptions for ideal CSTR, the age function should be given by equation (5). The average residence time,  $\bar{t}$ , that appears in equation (5) is found using equation (6). Substitution of equation (6) into equation (5) leads to equation (7) for the age function of an ideal CSTR that corresponds to the tested reactor. That age function is also plotted in Figure 1.

$$F_{CSTR}(\lambda) = 1 - \exp\left\{-\frac{\lambda}{\bar{t}}\right\} \quad (5)$$

$$\bar{t} = \frac{V}{\dot{V}} = \frac{10 \text{ L}}{20.2 \text{ L min}^{-1}} = 0.495 \text{ min} \quad (6)$$

$$F_{CSTR}(\lambda) = 1 - \exp\left\{-\frac{\lambda}{0.495 \text{ min}}\right\} \quad (7)$$

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.

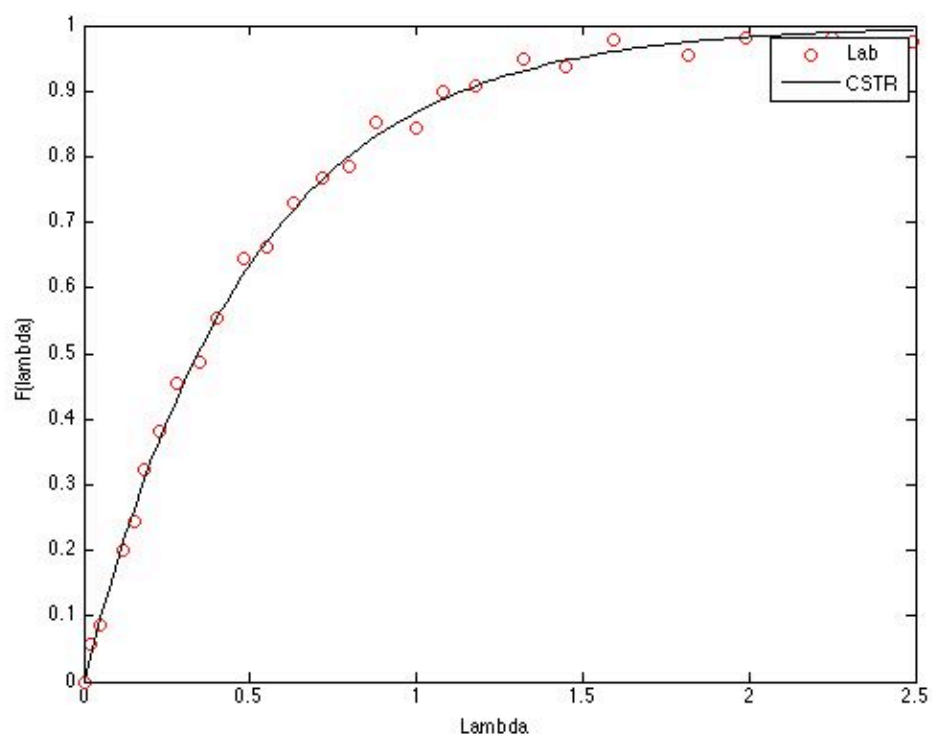


Figure1. Comparison of the experimental and ideal age functions.