A First Course on Kinetics and Reaction Engineering

Example 11.3

Problem Purpose

This problem illustrates the use of the age function measured using a step change stimulus to test whether a reactor conforms to the assumptions of the ideal CSTR model.

Problem Statement

A step change stimulus was used to characterize the flow in a 50 cm^3 stirred tank reactor. Pure water was flowing at a rate of 100 cm^3 min^{-1} when suddenly a tracer was added to the feed at a concentration of 3 mg cm^{-3}. The outlet concentration was measured as a function of time as recorded below. Is it safe to model this reactor as perfectly mixed?

Time (min)	***Conc. (mg cm^{-3})***
0	0.00
0.1	0.08
0.2	0.39
0.3	0.63
0.4	0.95
0.5	1.15
0.6	1.37
0.7	1.63
0.8	1.83
0.9	2.03
1	2.32
1.1	2.39
1.2	2.38
1.3	2.57
1.4	2.55
1.5	2.66
1.6	2.80
1.7	2.80
1.8	2.78
1.9	2.78
2	2.80

Problem Analysis

This problem provides data that can be used to calculate the age function for a laboratory reactor. The result can be compared to the age function that would be expected if the laboratory reactor behaved according to the ideal CSTR model.

Problem Solution

The problem states that a step change stimulus was applied to the reactor. Prior to the step change, the tracer mass concentration, C_0, was equal to zero, and after the step change the tracer mass concentration, C_f, was equal to 3 mg cm^{-3}. The times listed in the data column are equal to λ, the time elapsed since the imposition of the step change. The age function, $F(\lambda)$, can be computed from the response to a step change stimulus using equation (1).

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

In equation (1), the response is assumed to have been measured in the form of mass fractions, w, but here we have mass concentrations. A mass fraction can be converted to a mass concentration using equation (2). If we assume the amount of tracer was sufficiently small that the density of the fluid is equal to that of pure water after the step change, substitution of equation (2) into equation (1) gives an expression for the age function in terms of mass concentrations, equation (3). In equation (3), the concentrations, C_t, are the measured outlet concentrations at the times the response was measured, and as noted above, these times are equal to λ. Thus, for each row in the data table a value of $F(\lambda)$ for the laboratory reactor can be calculated. This can be done manually, using a spreadsheet or using mathematics software.

$$w_i = \frac{C_i}{\rho_{fluid}} \tag{2}$$

$$F(\lambda = t) = \frac{\dfrac{w_t}{\rho_{fluid}} - \dfrac{w_0}{\rho_{fluid}}}{\dfrac{w_f}{\rho_{fluid}} - \dfrac{w_0}{\rho_{fluid}}} = \frac{C_t - C_0}{C_f - C_0} \tag{3}$$

We wish to compare the experimental age function to that for a corresponding ideal CSTR. For an ideal CSTR, the age function is given by equation (4). The average residence time, $\overline{t}$, that appears in equation (4) is found using equation (5).

$$F_{CSTR}(\lambda) = 1 - \exp\left\{\frac{-\lambda}{\overline{t}}\right\} \tag{4}$$

$$\bar{t} = \frac{V}{\dot{V}} \tag{5}$$

The problem statement gives the values of the volume (V = 50 cm^3) and the volumetric flow rate ($\dot{V} = 100$ cm^3 min^{-1}), so equation (4) can be calculated for any value of λ.

In order to test whether the laboratory reactor obeys the assumptions of an ideal CSTR, the values of $F(\lambda)$ calculated for the laboratory reactor using equation (3) can be plotted as a function of λ. On the same set of axes, the CSTR age function, calculated using equation (4), can also be plotted. The resulting plots are shown in Figure 1. The figure shows that the experimental data deviate significantly from the values expected for an ideal CSTR, so the reactor should not be modeled as an ideal CSTR.

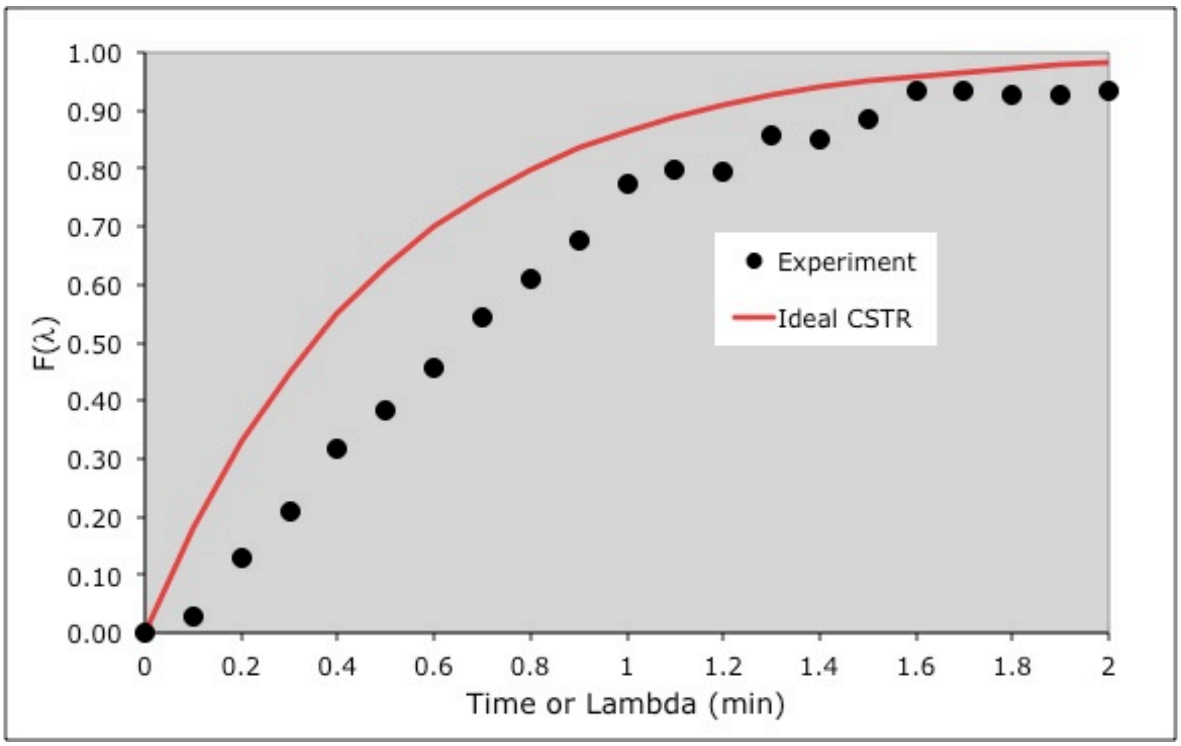

Figure1. Comparison of the experimental and ideal age functions.