A Simple Method For Derivation of Concentration Transfer Functions for Flow Systems with First Order Chemical Reaction

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The usual method of deriving the transfer function involves several steps relating outlet to inlet reactant concentrations in a flow system where chemical reaction occurs. An element of volume is chosen, and a differential balance is written. This takes into account mass transport due to convection and to whatever dispersive mechanism is assumed to operate in the system, as well as changes in mass due to the chemical reaction. The resulting differential equation is then Laplace transformed, taking initial and boundary conditions into account, and the ratio of transformed outlet to inlet concentrations is formed.

A convenient short cut is available if the reaction which occurs is first order. Let the elementary reaction

$$A \xrightarrow{k_1} P$$

occur in a flow system. If a mass balance on A is made in rectangular coordinates, by use of a volume element $dx\, dy\, dz$, the result is

$$\frac{\partial C_A}{\partial t} = -\frac{\partial(U_x C_A)}{\partial x} - \frac{\partial(U_y C_A)}{\partial y} - \frac{\partial(U_z C_A)}{\partial z} - k_1\, C_A + \phi(x, y, z, C_A) \quad (1)$$

where $\phi(x, y, z, C_A)$ represents all terms which account for mass transport other than the terms due to convection and reaction.

Evaluating Equation (1) at the steady state, subtracting the result from Equation (1), and defining the deviation variable

$$Y_A = C_A(x, y, z, t) - C_A(x, y, z, 0) \quad (2)$$

one obtains

$$\frac{\partial Y_A}{\partial t} = -\frac{\partial(U_x Y_A)}{\partial x} - \frac{\partial(U_y Y_A)}{\partial y} - \frac{\partial(U_z Y_A)}{\partial z} - k_1\, Y_A + \phi(x, y, z, Y_A) \quad (3)$$

Laplace transforming with respect to time, recognizing the initial condition $Y_A = 0$ at $t = 0$, and solving for $\overline{Y_A}$ one gets

$$\overline{Y_A} = \frac{1}{s + k_1}\left[\phi(x, y, z, \overline{Y_A}) - \frac{\partial(U_x \overline{Y_A})}{\partial x} - \frac{\partial(U_y \overline{Y_A})}{\partial y} - \frac{\partial(U_z \overline{Y_A})}{\partial z}\right] \quad (4)$$

Here $\phi(x, y, z, Y_A)$, the dispersion function in deviation form, contains Y_A and derivatives of Y_A with respect to x, y, and z, and if physical properties of the system do not change with time, then time does not appear in ϕ and s does not appear in its transform. Equation (4) can be solved for $\overline{Y_A}$ by using the boundary conditions appropriate to the system, one of which is

$$Y_A(a, b, c, t) = Y_i(t) \quad (5)$$

where a, b, and c are the values of x, y, and z at which the forcing function $Y_i(t)$ is introduced. From the result, the transfer function $\overline{Y_A}/\overline{Y_i}$ can be formed.

If no chemical reaction occurs in the system, then $k_1 = 0$, and from Equation (4) it is apparent that

$$\left[\frac{\overline{Y_A}}{\overline{Y_i}}\right]_{\substack{\text{reaction}\\ \text{occurring}}} = \left[\left(\frac{\overline{Y_A}}{\overline{Y_i}}\right)_{\text{no reaction}}\right]_{s \to s + k_1} \quad (6)$$

Thus for time-invariant physical properties, the concentration transfer function of a linear lumped or distributed parameter flow system in which a first-order irreversible chemical reaction occurs may be derived from the concentration transfer function for the same system with no reaction taking place. It is necessary merely to substitute $s + k_1$ for s. Since the transfer functions of a large number of dispersive systems with a wide variety of boundary conditions have already been derived (*1* to *4*) this method will allow the evaluation of these systems, when used as a chemical reactor with first-order kinetics, in a much simpler manner than by rederivation of their dynamic behavior from first principles.

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NOTATION

a, b, c = spatial coordinates at point system is forced
C_A = concentration of A
D_x, D_y, D_z = eddy dispersion coefficient
k_1 = reaction velocity constant
s = Laplace transform complex variable
U_x, U_y, U_z = average velocities
x, y, z = spatial coordinates
Y_A = concentration of A in deviation form
Y_i = concentration forcing function in deviation form
ϕ = terms in differential mass balance accounting for all mass fluxes of other than convective and reactive natures; that is, $\phi = 0$ for plug flow and complete mixing mechanisms, $\phi = \frac{\partial}{\partial x}\left(D_x \frac{\partial C_A}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C_A}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_A}{\partial z}\right)$ for eddy dispersion mechanism, etc.

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