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NOTE

Model for Time Lag in Signal Concentration for Product Removal in a One-Dimensional Column

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INTRODUCTION

A signal can be propagated through a chemical system to cause a change to occur. This signal can be concentration (solute or pH, for example), temperature, or pressure. The signal normally does not change in strength but serves to turn the system "on/off." Based on signal strength, the chemical system can produce, release, and/or remove some chemical species.

The specific example presented here is insulin release due to a change in glucose concentration. The glucose provides the signal to the pancreatic cells. The insulin has a self-inhibiting effect. This provides a self-regulating mechanism for the insulin concentration.

The system is shown in Fig. 1. Two configurations are illustrated. In Fig. 1(a) the cells are located in the flow path. In Fig. 1(b) the cells are located external to the flow path. There is communication between the flow path and the pancreatic cells through a permeable wall.

In either case, a step change in signal concentration is propagated through the system. The product production rate can be written as (*1*):

$$\dot{C} = k_p G - k_I C \tag{1}$$

The rate expression takes into account the production stimulated by the signal concentration and the self-inhibition of the product.

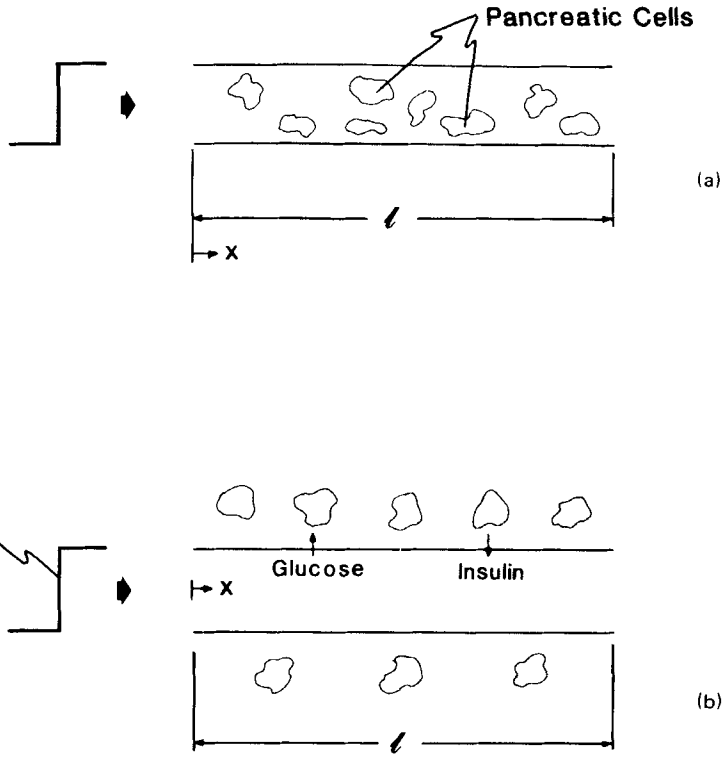

FIG. 1. System schematic: (a) cells in flow path, (b) cells external to flow path.

There can be a lag between the signal concentration in the bulk flow and the signal concentration that the cell senses. This can be due to mass transfer resistances across the cell and/or channel wall. This lag can be approximated by an exponential delay.

The purpose of this paper is to introduce a model which can account for an exponential lag in signal stimulus to produce a product. The production rate contains a term to account for self-inhibition by the product. This result can be used in many chromatographic mode processes (especially biological processes) where signal stimulus and self-inhibition are present.

MODEL

The processes is one whereby a signal concentration (C) is convected through the system (considered one-dimensional) (see Fig. 1). The signal

concentration causes the production of product (G) which has an inhibiting effect on the production rate. The signal concentration experiences a lag between the bulk concentration and the concentration that stimulates product.

The governing differential equation for a step change in signal concentration is

$$\frac{\partial C}{\partial t} + \nu \frac{\partial C}{\partial x} = (G_1 - G_0)[1 - e^{-k_D(t-x/\nu)}]u\left(t - \frac{x}{\nu}\right) - k_I C + k_P G_0 \qquad (2)$$

The reaction equilibria are such that

$$k_I C_0 = k_p G_0 \qquad \text{(initial state)}$$

$$k_I C_1 = k_p G_1 \qquad \text{(final state)}$$

The initial and boundary conditions are

$$t = 0, \qquad C = C_0$$

$$x = 0, \qquad C = C_0$$

The following dimensionless variables are introduced:

$$\phi = \frac{C - C_0}{C_1 - C_0}$$

$$\tau = k_I t$$

$$X_c = k_I X/\nu$$

$$K = k_D/k_I$$

Equation (2) becomes

$$\frac{\partial \phi}{\partial \tau} + \frac{\partial \phi}{\partial X_c} = 1 - e^{-K(\tau - X_c)}u(\tau - X_c) - \phi \qquad (3)$$

$$\tau = 0, \qquad \phi = 0$$

$$X_c = 0, \qquad \phi = 0$$

The solution is

$$\phi = [1 - e^{-X_c}][1 - e^{-K(\tau - X_c)}]u(\tau - X_c) \tag{4}$$

Some limiting cases can be checked. When $K = 0$, there is no signal stimulus ($k_p = 0$). For this case, Eq. (4) yields $\phi = 0$, which indicates no product.

For $k \to \infty$, there is no lag in the signal stimulus. Equation (4) becomes

$$\phi = [1 - e^{-X_c}]u(\tau - X_c) \tag{5}$$

This is also the solution to Eq. (3) for no signal lag. Since there is no lag, a steady-state profile is developed instantaneously behind the advancing front (see Fig. 2). The exponential rise is due to balance between signal concentration, product concentration, and convective flux of product.

As $t \to \infty$, the lag disappears and the solution becomes Eq. (5). This makes sense as the above arguments were based on the disappearance of the signal lag.

Some sample results are shown in Figs. 3 and 4. Figure 3 shows the product axial profiles as a function of time. Compare these results with Fig. 2. When the front just reaches a given X_c, Eq. (5) gives $\phi = 1 - e^{-X_c}$. Equation (4) gives $\phi = 0$. Another view of the lag effect is shown in Fig. 4. The product concentration at a given position in Fig. 3 is shown for both a lag and no lag case. The exponential rise of the product concentration shows the lag effect.

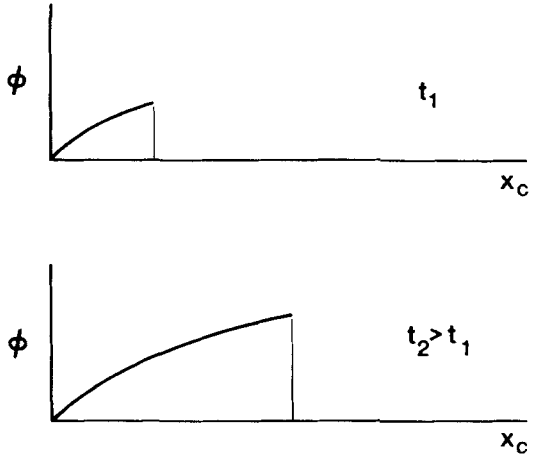

FIG. 2. Steady-state profiles with no lag.

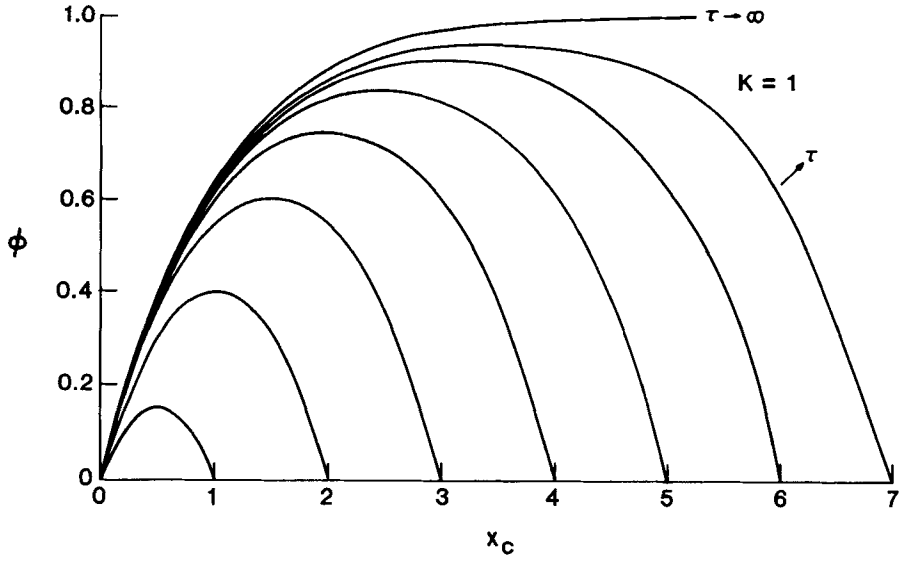

FIG. 3. Axial profiles as a function of time.

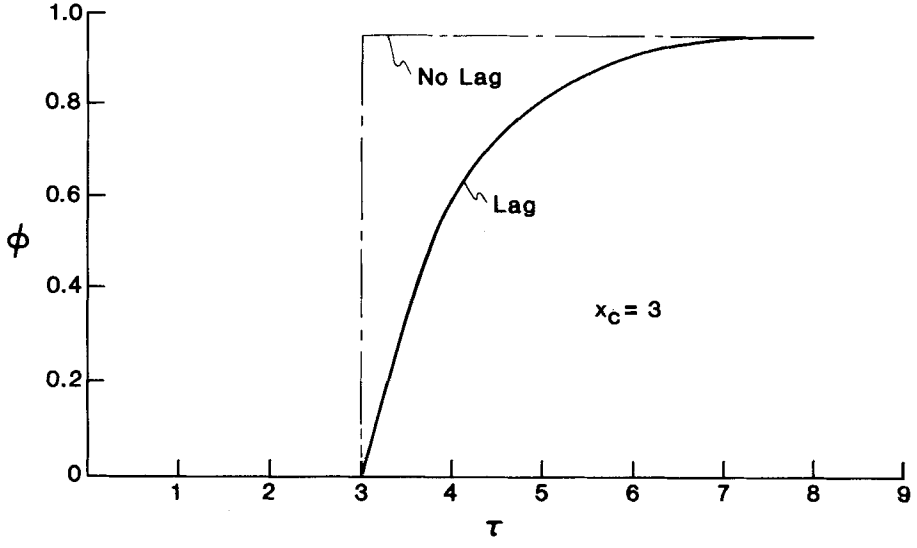

FIG. 4. Concentration profile as a function of time for a given position.

This result can also be used to estimate system properties. k_I, the inhibition constant, can be determined as follows. Change the axial velocity v (this changes X_c for a given position). Measure the steady-state value of ϕ, ϕ_{ss}, for various v. Using Eq. (5), plot ln $(1 - \phi_{ss})$ vs x/v. The slope will be k_I. If C_1 is unknown, then obtain the following rates for two different velocities:

$$\frac{\phi_{ss_1}}{\phi_{ss_2}} = \frac{1 - e^{-k_I x/v_1}}{1 - e^{-k_I x/v_2}} \tag{6}$$

The only unknown is k_I since the $C_1 - C_0$ cancels in the numerator and denominator.

An alternative form of Eq. (4) is

$$\phi/\phi_{ss} = 1 - e^{-k(\tau - X_c)}u(\tau - X_c) \tag{7}$$

since $\phi_{ss} = 1 - e^{-X_c}$. So, a plot of ln $(1 - \phi/\phi_{ss})$ vs $(\tau - X_c)$ has a slope of K. Since k_I is now known, k_D can be estimated.

k_p can be estimated using the reaction equilibria criteria $k_p G_0 = k_I C_0$.

The validity of the model for a particular application can be verified by the above plots. Ln $(1 - \phi/\phi_{ss})$ vs $(\tau - X_c)$ and ln $(1 - \phi_{ss})$ vs x/v should be linear.

One interesting point should be noted. If a Dirac delta function is used instead of a step function for the signal concentration, the result is $\phi = 0$ for all x and τ (*2*). This concentration only passes a particular point for an instant. The lag prevents any possibility for increased signal strength in the cells and, therefore, no production.

CONCLUSIONS

A model has been presented which allows for a lag in signal concentration to producing cells. The product can also be self-inhibiting. The effect of the lag on column profiles and exit concentrations has been shown. Several methods for estimating the parameters and verifying the model were discussed.

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