Batch to fed batch system

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1 Introduction

This is the description of how to derive the mass balance of a fed-batch bioreactor, given the mass balance of the batch system. A fed-batch system of biodiesel production using microalgae is demonstrated as an example[?]

2 Batch system

The mass balance of the batch system is shown as below:

$$\frac{dX}{dt} = \mu_0 X - \mu_d X \tag{1}$$

$$\frac{dN}{dt} = -\mu N \cdot \frac{N}{N + K_N} \cdot X \tag{2}$$

$$\frac{dq}{dt} = \mu_N \cdot \frac{N}{N + K_N} - (\mu_0 - \mu_d) \cdot q \tag{3}$$

$$\frac{df}{dt} = \mu_0(\theta \cdot q - \epsilon \cdot f) - \gamma \cdot \mu_N \frac{N}{N + K_N} + \mu_d \cdot \epsilon \cdot f \tag{4}$$

$$\mu_0 = g(X, q, I_0) \tag{5}$$

The system above is the structure of hybrid model that contains 4 state variables: X, N, q, f. Eq. 5 represents the data-driven equations of the hybrid model, which takes the concentration of X, q and the control variable I_0 as inputs. The goal of Eq. 5 is to predict μ as a time-varying variable through the whole process.

3 Fed-batch system

To start with, for all state variables in the fed-batch system without direct feeding streams, the mass balance can be represented as the following form:

$$\frac{d(CV)}{dt} = V r_c(C, \mu) \tag{6}$$

Where C is the concentration of the state variable (g/L), V is the volume of the feed stream that being added to the bioreactor (L), r_c is the reaction rate of state variable C $(g/(L \cdot h))$, which is the function of the state variable C and the control variable μ.

On the other hand, the general mass balance of the state variable which is fed to the biosystem directly, the mass balance can be represented as below:

$$\frac{d(SV)}{dt} = F_{in}S_{in} + Vr_s(S, \mu) \tag{7}$$

Where F_{in} $(L/h)$is the volumetric flowrate that being fed to the system. Therefore, the change of the volume is shown as below:

$$F_{in} = \frac{dV}{dt} \tag{8}$$

Therefore, Eq. **??** and Eq. 7 can be further derived through the chain rule of the differential calculus:

$$\frac{d(CV)}{dt} = C\frac{dV}{dt} + V\frac{dC}{dt} = V\frac{dC}{dt} + F_{in}C \tag{9}$$

$$\frac{d(SV)}{dt} = S\frac{dV}{dt} + V\frac{dS}{dt} = V\frac{dS}{dt} + F_{in}S \tag{10}$$

Furthermore, by substituting Eq. 6 to Eq. 9 and Eq. **??** to Eq. 10, we can obtain the following mass balance equations:

$$\frac{dC}{dt} = -\frac{F_{in}}{V}C + r_c(C, \mu) \tag{11}$$

$$\frac{dS}{dt} = -\frac{F_{in}}{V}(S - S_{in}) + r_s(S, \mu) \tag{12}$$

Now, we can start to drive the mass balance of the fed-batch system given Eq 1 to Eq. 4.

$$\begin{aligned}
\frac{d(XV)}{dt} &= Vr_X(X) \\
\frac{dX}{dt}V + \frac{dV}{dt}X &= Vr_X(X) \\
\frac{dX}{dt}V &= -\frac{dV}{dt}X + Vr_X(X) \\
\frac{dX}{dt} &= -\frac{F_{in}}{V}X + r_X(X) \\
\frac{dX}{dt} &= -\frac{F_{in}}{V}X + (\mu_0 X - \mu_d X)
\end{aligned}$$

$$
\begin{aligned}
\frac{d(NV)}{dt} &= F_{in}N_{in} + Vr_N(N) \\
\frac{dN}{dt}V + \frac{dV}{dt}N &= F_{in}N_{in} + Vr_N(N) \\
\frac{dN}{dt}V + F_{in}N &= F_{in}N_{in} + Vr_N(N) \\
\frac{dN}{dt}V &= F_{in}(N_{in} - N) + Vr_N(N) \\
\frac{dN}{dt} &= \frac{F_{in}(N_{in} - N)}{V} + r_N(N) \\
\frac{dN}{dt} &= \frac{F_{in}(N_{in} - N)}{V} - \mu N \cdot \frac{N}{N + K_N} \cdot X
\end{aligned}
$$

The derivation of the mass balance of q needs to be modified since q is the intracellular concentration of nitrate. Therefore, the concentration is not directly impacted by the feeding of nitrate. Thus, the mass balance of q is derived considering the mass balance between q and N. As pointed out from the literature, the nitrate consumption rate must be equal to the accumulation of the intracellular nitrogen:

$$
\frac{d(X \cdot q)}{dt} = -\frac{dN}{dt} \tag{13}
$$

Therefore, the following equations can be derived:

$$
\begin{aligned}
\frac{d(X \cdot q)}{dt} &= -\frac{dN}{dt} \\
\frac{dq}{dt}X + \frac{dX}{dt}q &= -\frac{dN}{dt} \\
\frac{dq}{dt}X &= -\frac{dN}{dt} - \frac{dX}{dt}q \\
\frac{dq}{dt} &= -\frac{\frac{dN}{dt}}{X} - \frac{dX}{dt}\frac{q}{X} \\
\frac{dq}{dt} &= -[\frac{F_{in}(N_{in} - N)}{V} - \mu_N \cdot \frac{N}{N + K_N} \cdot X] \cdot \frac{1}{X} - [-\frac{F_{in}}{V}X + (\mu_0 - \mu_d)X]\frac{q}{X} \\
\frac{dq}{dt} &= -\frac{F_{in}(N_{in} - N)}{VX} + \mu_N \cdot \frac{N}{N + K_N} + \frac{F_{in}q}{V} - (\mu_0 - \mu_d)q
\end{aligned}
$$

The derivation of product f is derived following different procedure. As pointed out by literature, the reaction rate of f is derived as the difference between biolipid synthesis and consumption, respectively. Thus, the mass balance of f keeps the same as the batch system:

$$
\frac{df}{dt} = \mu_0(\theta \cdot q - \epsilon \cdot f) - \gamma \cdot \mu_N \frac{N}{N + K_N} + \mu_d \cdot \epsilon \cdot f \tag{14}
$$

In summary, the mass balance of the fed batch bioreactor of the hybrid model can be illustrated as below:

$$\frac{dX}{dt} = -\frac{F_{in}}{V}X + (\mu_0 X - \mu_d X) \tag{15}$$

$$\frac{dN}{dt} = \frac{F_{in}(N_{in} - N)}{V} - \mu N \cdot \frac{N}{N + K_N} \cdot X \tag{16}$$

$$\frac{dq}{dt} = -\frac{F_{in}(N_{in} - N)}{VX} + \mu_N \cdot \frac{N}{N + K_N} + \frac{F_{in} q}{V} - (\mu_0 - \mu_d)q \tag{17}$$

$$\frac{df}{dt} = \mu_0(\theta \cdot q - \epsilon \cdot f) - \gamma \cdot \mu_N \frac{N}{N + K_N} + \mu_d \cdot \epsilon \cdot f \tag{18}$$

$$F_{in} = \frac{dV}{dt} \tag{19}$$

$$\mu_0 = g(X, q, I_0) \tag{20}$$