Advection–diffusion constrained metabolic reaction in bioreactor analysis for hydrogen production

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ABSTRACT

The reaction advection–diffusion equation (RADE) is proposed to describe the dynamic processes in a heterogeneous biochemical system involved in hydrogen production in a photobioreactor. The spatial- and temporal-dependent concentration functions of metabolites in the differential equation are assumed as a multiplication of the spatial-dependent function and the temporal-dependent function such that RADE can be uncoupled into spatial-dependent advection–diffusion equation and the kinetics equation. The advection–diffusion equation along with the boundary conditions of the photobioreactor acts as a constraint in solving the kinetics equation. Such a decomposition leads to an approximate analytical solution of the advection–diffusion equation for a batch mode tubular photoreactor under solar radiation. As a constraint, the analytical solution of the advection–diffusion equation is then introduced into the kinetics equation to obtain the dynamics of the concentration of metabolites in an inhomogeneity system. The dynamics of the biochemical processes in a photobioreactor, as an example, was studied and the production of H_2 at the mesh grids was calculated for 250 h operation under solar radiation. The results demonstrate the variation of H_2 in both the radial and the angular directions with time. The perturbed dynamics of hydrogen production is consistent in trend with the available experimental observations of H_2 production in outdoor photobioreactors.

1. Introduction

Most of the mathematical models describing biochemical processes, e.g., Metabolic Control Theory [1–3] and Biological System Theory [4] assume that the system is homogeneous and the reaction takes place instantaneously throughout the space of the system and therefore, advection and diffusion of the reactants and the products as well as the effects of the boundary conditions can be ignored. For a small scale system, such as small laboratory test apparatus where the homogeneity and the optimum microenvironment of the system could be conveniently monitored and maintained, the homogeneous assumption holds well. For industrial scale systems, e.g., bioreactors in which the mixture of biomass, biocatalysts, and nutrients are not uniform even under constantly mechanical mixing and the homogeneity and the optimum microenvironment are hardly obtainable [5,6], the homogeneous assumption may lead to discrepancies in the outcomes when compared with a small scale system. A typical example is the photobioreactor (PBR) for biomass or hydrogen (H_2) production. When a PBR operates under sunlight, the incident light intensity illuminated on the reactor external surface is inhomogeneous and varies with time. In addition, the sunlight is absorbed by biomass as it passes through the culture, which results in the light attenuation (or light gradient) across the medium in the PBR. These lead to the distribution of O_2 and H_2 at the boundary of as well as within the reactor being inhomogeneous and time-dependent. Thus, PBR is an

inhomogeneous system that has to be considered in the reactor design and optimization and in the prediction of H_2 production. The inhomogeneity is also one of the issues in widely recognized scaleup problem [6–8] that prohibits commercialization of the production of biomass, biofuel, or H_2. Most of the methods for PBR analysis and design are based on the averaged sunlight intensity to calculate biomass or H_2 production [9,10]. Such a simplification could either under- or over-estimate H_2 production due to the inhomogeneity on the boundary and in the system. To understand the effect of inhomogeneity on the production of biomass or H_2 in a PBR and to improve and optimize PBR design, we propose to use the reaction advection–diffusion equation (RADE) to describe the inhomogeneity and dynamics of the biochemical processes. To facilitate in solving the spatial- and temporal-dependent partial differential equation, RADE, we assume the concentration of metabolites involving in the biochemical process can be expressed as the multiplication of a time-dependent and a spatial-dependent functions such that the original partial differential equation can be decoupled into the spatial-dependent advection–diffusion equation and the kinetics equation, which makes the analytical solution tractable. The advection–diffusion equation can be considered as a constraint in solving the kinetics equation. A tubular PBR under the sunlight illumination is studied and the effect of the inhomogeneity on the H_2 production is demonstrated. The proposed mathematical model provides a valuable and an economic computational tool for the optimization of PBR design and the improvement of the efficiency of light utilization by biomass.

2. Governing equations

For inhomogeneous biochemical systems, e.g., PBR, both physical and chemical processes play important roles in the final products. The physical process involved is mass transport through advection and diffusion while the chemical process is the kinetics of different metabolites converting to each other. The mathematical model describing the inhomogeneous system is reaction advection–diffusion equation given by (see Ref. [11])

$$\frac{\partial C_i}{\partial t} + U \cdot \nabla C_i = \nabla \cdot (D_i \nabla C_i) + R_i \quad (i = 1, 2, 3, \cdots, N) \tag{1}$$

where i denotes ith component; $C_i(\vec{x}, t)$ is the concentration function of spatial position $\vec{x}$ and time t; U is the average velocity of fluid flow determined by the Navier–Stokes equations; D_i is the diffusion coefficient; and R_i accounts for all the local biochemical reactions; ∇ is the gradient operator.

Numerous theories such as Biological System Theory (BST) [4], Metabolic Control Theory (MCT) [1–3], among others have been developed to describe the kinetics of biochemical reactions. Here we use BST (S-system or power-law formalism, though other laws will work the same way) [4] to define R_i in Eq. (1), i.e.,

$$R_i(t) = \alpha_i \prod_{j=1}^{n+m} C_j^{g_{ij}} - \beta_i \prod_{j=1}^{n+m} C_j^{h_{ij}} \tag{2}$$

where α_i and β_i are the rate constants; g_{ij} and h_{ij} are the kinetic orders. Eq. (1) can then be written as

$$\frac{\partial C_i}{\partial t} + U \cdot \nabla C_i = \nabla \cdot (D_i \nabla C_i) + \alpha_i \prod_{j=1}^{n+m} C_j^{g_{ij}} - \beta_i \prod_{j=1}^{n+m} C_j^{h_{ij}} \tag{3}$$

$$(i = 1, 2, 3, \cdots, N).$$

By assuming that $C_i(\vec{x}, t)$ can be represented by a multiplication of spatial-dependent function $X_i(\vec{x})$ and time-dependent function $T_i(t)$, i.e., $C_i(\vec{x}, t) = X_i(\vec{x})T_i(t)$, Eq. (3) can then be written as

$$\frac{\dot{T}_i(t)}{T_i(t)} = \frac{\nabla \cdot (D_i \nabla X_i(\vec{x}))}{X_i(\vec{x})} - \frac{U \cdot \nabla X_i(\vec{x})}{X_i(\vec{x})} + \frac{1}{X_i(\vec{x})T_i(t)} \left[\alpha_i \prod_{j=1}^{n+m} C_j^{g_{ij}} - \beta_i \prod_{j=1}^{n+m} C_j^{h_{ij}} \right]$$

$$(i = 1, 2, 3, \cdots, N). \tag{4}$$

Now, let the advection–diffusion term to be zero, i.e.,

$$\frac{\nabla \cdot (D_i \nabla X_i(\vec{x}))}{X_i(\vec{x})} - \frac{U \cdot \nabla X_i(\vec{x})}{X_i(\vec{x})} = 0, \tag{5}$$

Savageau's power-law [4], Eq. (2), is recovered from Eq. (4), i.e.,

$$\dot{T}_i(t) = \frac{1}{X_i(\vec{x})} \left[\alpha_i \prod_{j=1}^{n+m} C_j^{g_{ij}} - \beta_i \prod_{j=1}^{n+m} C_j^{h_{ij}} \right] \tag{6}$$

with the only difference being that the concentration function is both spatial- and temporal-dependent. $X_i(\vec{x})$ in Eq. (6) has to be determined by solving Eq. (5) in combination with the given boundary conditions of a system.

The homogeneous advection–diffusion equation, Eq. (5), used here is only for a special case. In general, the advection–diffusion equation can be described in three forms, i.e.,

$$\frac{\nabla \cdot (D_i \nabla X_i(\vec{x}))}{X_i(\vec{x})} - \frac{U \cdot \nabla X_i(\vec{x})}{X_i(\vec{x})} = \begin{cases} 0 \\ \text{constant} \\ f(X_i(\vec{x})). \end{cases} \tag{7}$$

Consequently, the kinetic equations in Eq. (6) become

$$\dot{T}_i(t) = \frac{1}{X_i(\vec{x})} \left[\alpha_i \prod_{j=1}^{n+m} C_j^{g_{ij}} - \beta_i \prod_{j=1}^{n+m} C_j^{h_{ij}} \right] + \begin{cases} 0 \\ \text{constant} \times T_i(t) \\ f(X_i(\vec{x}))T_i(t). \end{cases} \tag{8}$$

The use of different forms of the advection–diffusion equation in Eq. (7) depends on the state of the source in a system. The dependence of the concentration on spatial position in the kinetic equations could be valuable in the analysis of inhomogeneous biochemical systems, e.g., in PBRs, in which light attenuation results in the inhomogeneous distribution of concentration of various constituents.

3. Solution of the governing equations

3.1. Analytical solution of advection–diffusion equation

For a PBR, the intensity of incident solar radiation on its surface varies with time and spatial position. The boundary condition for the advection and diffusion equation is therefore both temporal- and spatial-dependent. Here, we consider a batch mode tubular PBR with the boundary conditions at two ends being independent of the spatial position and on the cylindrical surface varying with time and spatial position as