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A multiphase mixture model for substrate concentration distribution characteristics and photo-hydrogen production performance of the entrapped-cell photobioreactor

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HIGHLIGHTS

- A multiphase mixture model is developed for the entrapped-cell photobioreactor.
- Substrate concentration distribution and photo-hydrogen production are predicted.
- Interaction mechanism between biochemical reaction and transfer process is revealed.
- The effects of difference operation parameters are investigated.

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ABSTRACT

A multiphase mixture model was developed for revealing the interaction mechanism between biochemical reactions and transfer processes in the entrapped-cell photobioreactor packed with gel granules containing *Rhodopseudomonas palustris* CQK 01. The effects of difference operation parameters, including operation temperature, influent medium pH value and porosity of packed bed, on substrate concentration distribution characteristics and photo-hydrogen production performance were investigated. The results showed that the model predictions were in good agreement with the experimental data reported. Moreover, the operation temperature of 30 °C and the influent medium pH value of 7 were the most suitable conditions for photo-hydrogen production by biodegrading substrate. In addition, the lower porosity of packed bed was beneficial to enhance photo-hydrogen production performance owing to the improvement on the amount of substrate transferred into gel granules caused by the increased specific area for substrate transfer in the elemental volume.

1. Introduction

Biological hydrogen production is a safe, economical and sustainable way for producing hydrogen owing to these advantages of its environmentally compatibility as well as the ability to overcome environmental pollution and high cost of equipment investment (Azwar et al., 2014; Redwood et al., 2012). Among these microorganisms being employed for biological hydrogen production, photosynthetic bacteria (PSB) is recognized as an attractive candidate because of its high theoretical conversion yield and the capability of eliminating the oxygen inactivation of biological systems caused by oxygen-evolving activity (Adessi and De Philippis, 2014; Basak et al., 2014a; Guo et al., 2014). Moreover, PSB can not only utilize a wide range of solar spectrum but also biodegrade a great variety of organic substrates for achieving waste treatment (Basak et al., 2014b; Chitapornpan et al., 2013; Prachanurak et al., 2014). As a result, many researchers have paid their attention to this area all over the world.

At present, many studies on photo-hydrogen production by PSB are carried out in the suspended-cell photobioreactor due to the good mass transfer (Cai and Wang, 2014; Obeid et al., 2009). Nevertheless, it should be pointed out that the suspended-cell photobioreactor is difficult to achieve higher cell concentration and efficient solid–liquid separation (Li et al., 2013; Olivieri et al., 2014). Immobilized-cell techniques, including cell entrapment, biofilm and self-flocculation, are promising technologies because

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of the increases of cell concentration and operation stability as well as the enhancements of volumetric productivity and ability to recover and reuse cell mass (Guo et al., 2011; Murphy and Berberoglu, 2014; Zagrodnik et al., 2013). In particular, the cell entrapment seems to be a more reasonable way because it can provide a stable and favorable environment for the growth of PSB entrapped by gel granule (Wang et al., 2013, 2010). Note that, the multiphase flow and mass transfer as well as biochemical reactions exist simultaneously in the entrapped-cell photobioreactor, which affect substrate concentration distribution characteristics and photo-hydrogen production performance. Therefore, the detailed assessments of the complex biochemical reactions and transfer processes are beneficial to promote the scale-up application of photo-hydrogen production system. Unfortunately, it is very difficult to measure the multiphase flow and mass transfer as well as biochemical reactions in the entrapped-cell photobioreactor by experimental means.

As a powerful tool, the mathematical model can reveal the interaction mechanism between biochemical reactions and transfer processes. In recent years, many mathematical models have been established for the prediction of photo-hydrogen production. Zhang et al. (2013) developed a two-dimensional steady-state model for a novel annular fiber-illuminating biological hydrogen reactor to simulate the convection and diffusion of substrate in the bulk fluid zone as well as the diffusion and degradation of substrate in biofilm zone (Zhang et al., 2014). Yang et al. (2011) applied the lattice Boltzmann method to simulate a substrate solution flowing past a circular cylinder with biochemical reaction as well as a bioreaction system of substrate solution through a porous granule immobilized PSB (Liao et al., 2013). However, these methods have been not taken into account the complex multiphase flow and mass transfer in the photobioreactor. More recently, a two-phase flow and mass transfer model was proposed to predict the substrate biodegradation and photo-hydrogen production (Liao et al., 2011). Unfortunately, in the previous work, the studies on substrate concentration distribution characteristics and photo-hydrogen production performance of the entrapped-cell photobioreactor have not been reported.

In the present work, a multiphase mixture model is developed and the numerical simulation results are validated using the experimental data reported by Wang et al. (2010). Meanwhile, the photo-hydrogen production performance of the entrapped-cell photobioreactor under various factors, including operation temperature, influent medium pH value and porosity of packed bed, are investigated. In addition, the substrate concentration distribution characteristics inside gel granule and mainstream channel are also explored in this work.

2. Model description

The entrapped-cell photobioreactor was a sealed vessel with a working volume of $0.1 \times 0.04 \times 0.2\ m^3$ and packed with gel granules (4 mm in diameter) containing PSB (*Rhodopseudomonas palustris* CQK 01). The substrate flow direction in mainstream channel and the products transfer direction inside gel granule are named as the *h*-direction and the *r*-direction, respectively. The glucose is used as the sole carbon source and the substrate medium is fed in the entrapped-cell photobioreactor by a peristaltic pump. And then, the glucose diffuses into gel granules from mainstream channel and is biodegraded by the entrapped cells via photoheterotrophic pathway under illumination conditions provided by LED lamps with main light wavelength of 590 nm and light intensity of 6000 lx. Finally, the produced gases and metabolites diffuse out of gel granules and are discharged out of the entrapped-cell photobioreactor by the flowing substrate medium. Obviously, the multiphase flow and mass transfer as well as biochemical reactions exist simultaneously in the entrapped-cell photobioreactor. For the numerical realization of the multiphase mixture model, in this work, the following assumptions were utilized:

(1) The entrapped-cell photobioreactor is used at the steady-state operating conditions.
(2) The transfer processes of substrate and products in mainstream channel are considered as one-dimensional flow along the *h*-direction.
(3) Thermal physical properties of fluids are assumed to be constant and the transfer processes of substrate and products can be described by Darcy's law.
(4) The biochemical reactions only occur inside gel granules.
(5) Considering the uniform distribution and activity of PSB inside gel granules.
(6) As the only gaseous products generated from substrate biodegradation, the mole ratio of hydrogen and carbon dioxide is 2:1 referring to Koku et al. (2002).

2.1. Governing equations

Based on the assumptions mentioned above, in this work, the multiphase flow and mass transfer processes in the entrapped-cell photobioreactor can be described using the multiphase mixture model presented by Wang and Cheng (1996).

The mass conservation in phase 'k' and multiphase mixture can be written as:

$$\nabla \cdot (\rho_k u_k) = \dot{m}_k \tag{1}$$

$$\nabla \cdot (\rho u) = \sum \dot{m}_k \tag{2}$$

where the subscript 'k' refers to the phase 'k'. ρ represents the density, kg/m^3; u the vector velocity, m/s; $\dot{m}_k$ the interfacial mass transfer rate from all other phase to phase 'k', kg/m^3/s.

The momentum conservation in phase 'k' and multiphase mixture can be written as:

$$\rho_k u_k = -\frac{K k_{rk}}{\nu_k}(\nabla p_k - \rho_k g) \tag{3}$$

$$\rho u = -\frac{K}{\nu}(\nabla p - \gamma_\rho \rho g) \tag{4}$$

where k_{rk} is the relative permeability of phase 'k'; g the gravitational force, m/s^2; ν the kinematic viscosity, m^2/s; K the absolute permeability, m^2; γ_ρ the density correlation factor, which can be defined as (Kaviany, 1995):

$$K = \frac{\varepsilon^3 r_{gr}^2}{45(1-\varepsilon)^3} \tag{5}$$

$$\gamma_\rho = \frac{\sum_k \rho_k \lambda_k}{\sum_k \rho_k s_k} \tag{6}$$

where ε is the porosity of packed bed; r_{gr} the radius of gel granule, m; s_k the saturation of phase 'k'. Meanwhile, λ_k represents the mobility of phase 'k' and can be calculated by Wang and Cheng (1996).

The conservation of species 's' in the multiphase mixture can be written as:

$$\nabla \cdot (\gamma_s \rho u \omega^s) = \nabla \cdot (\varepsilon \rho D^s \nabla \omega^s) + \nabla \cdot \left\{ \varepsilon \sum_k [\rho_k s_k D_k^s (\nabla \omega_k^s - \nabla \omega^s)] \right\} - \nabla \cdot \left(\sum_k \omega_k^s j_k \right) - \phi^s \tag{7}$$