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Predicting microalgae growth

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ABSTRACT

A generally applicable kinetic model is presented to predict light limited microalgal growth. This model combines a mathematical description for photoautotrophic sugar production with a description for aerobic chemoheterotrophic biomass growth. The model is based on five parameters which are directly measurable but were obtained from literature for the purpose of this study. The model was validated for *Chlorella sorokiniana* with 52 experiments derived from eight publications and for *Chlamydomonas reinhardtii* with 32 experiments derived from seven publications. The specific growth rate was initially predicted with a mean absolute percent error (MAPE) of 34–36%. The low accuracy is most likely caused by simplifications in the light model and inaccurate parameter estimations. When optimizing the light model per experimental dataset, a 1–2% MAPE was obtained. When optimizing input parameters separately from the light model, a 2–18% MAPE was realized. After validating this model on batch data, we conclude that this model is a reliable engineering tool to predict growth in photobioreactors provided the light field is accurately measured or calculated.

1. Introduction

Microalgae exploit photosynthesis to convert water and carbon dioxide into sugars by means of light energy. These sugars are subsequently used to support biomass growth. Microalgae growth in a photobioreactor can thus be calculated based on a model describing light-dependent sugar production by photosynthesis in combination with a model describing aerobic chemoheterotrophic growth on sugar. Ideally, the model parameters are all independently measurable in dedicated small-scale experiments in addition to the actual process to be predicted. In order to be suitable as a tool for photobioreactor engineers, the model should be as uncomplicated as possible while still including the most important reactions and providing sufficient accuracy.

Models that predict the light gradient include the Lambert–Beer Law, the radiative transfer equation (RTE), and a simplification of the two-flux model [1,2]. The Lambert–Beer Law is the simplest as it accounts only for light absorption but can be extended and improved by including light scattering [3]. The most dominant effect of light scattering is the increase in the light path travelled through the microalgae suspension increasing the probability of light absorption. This effect can be accounted for by modifying the attenuation coefficient. As such, it is possible to describe the light gradient with sufficient accuracy with the Lambert–Beer Law [4].

To describe photosynthesis, a model is required that describes the photosynthetic activity in response to light exposure. Photosynthetic activity increases linearly with light intensity under low light levels and then begins to stabilize towards a maximum photosynthetic rate at high light intensities. This trend is confirmed by the mechanistic description of photon absorption and utilization using a cumulative one-hit Poisson function [5] which results in the exponential model of Webb [6]. According to literature, the photosynthetic response, however, is best described by yet another hyperbolic function based on the hyperbolic tangent function [7]. As a result, the photosynthetic efficiency is maximal at low photon absorption rates and decreases slowly when approaching the maximal photosynthetic rate.

Sugar produced by photosynthesis in the chloroplast of the microalgae is used to support biomass growth. This growth metabolism is complex and can be described as aerobic chemoheterotrophic growth. Two general processes can be distinguished, i.e., the formation of new biomass and cellular maintenance (anabolism), which are both supported by aerobic respiration of sugars in the mitochondria (catabolism). The partitioning of sugar between anabolism and catabolism is described according to Pirt [8]. Pirt states that per biomass unit produced a fixed amount of sugar has to be respired, which is described by the biomass yield on sugar. Additionally a small amount of sugar is continuously respired providing energy for cellular maintenance.

Current light-limited microalgae growth models can be divided in photosynthesis- irradiance (PI) curve based models [3,9–12] and empirical models that are fitted to measured relations between specific growth rate and irradiance [13–15]. Although these models often include a respiratory term, Geider et al. [10] included a growth-related respiratory term. In reality, however, sugar is respired for energy to support cellular maintenance and anabolic reactions. Consequently, when neglecting this partitioning, respiration is often identified as energy loss.

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What is lacking in the current models used for engineering studies is a simple microalgae growth model which takes into account compartmentalization between chloroplast and mitochondria. The proposed model, therefore, differentiates between photosynthesis and respiration by combining the Lambert–Beer Law, Jassby and Platt [7], and Pirt [8]. With this strategy, differentiation is made between photosynthetically derived sugars used for: (1) cellular maintenance, (2) growth-related respiration, and (3) cell growth. The advantage of this differentiation is that the microalgae metabolism is more accurately represented while maintaining simplicity with the model formulation as much as possible and minimizing the number of parameters required.

In this study, an engineering model for microalgae growth in photobioreactors is introduced and validated with *Chlorella sorokiniana* and *Chlamydomonas reinhardtii*. The model input parameters can be measured with dedicated experiments. For the purpose of this study, the model input parameters are acquired from literature and include: molar mass of the microalgae (M_x); specific light absorption coefficient ($a_{x,\lambda}$); sugar yield on photons ($Y_{s/ph}$); biomass yield on sugar ($Y_{x/s}$); maintenance specific sugar consumption rate (m_s); maximal specific sugar production rate ($q_{s,m}$); and maximal specific growth rate (μ_m). In this manner, a robust evaluation of the model accuracy could be constructed. This is one of the few studies where one single microalgae growth model is employed to predict growth experiments of various studies under completely different conditions.

2. Theory

2.1. Growth model

2.1.1. Photoautotrophic sugar production

All of the sugar that is used for aerobic chemoheterotrophic biomass growth is produced by photoautotrophic sugar production. In our model, the photoautotrophic sugar production is represented by coupling photosynthesis and the Calvin–Benson cycle. Hereby, it is assumed that all energy generated in the form of ATP and NADPH during photosynthesis is used in the Calvin–Benson cycle to incorporate CO_2 into triose sugars.

The rate of photoautotrophic sugar production is dependent on light intensity (Eq. (1)). This equation is equivalent to the model of Jassby and Platt which is based on a hyperbolic tangent function [7]. The original equation proposed by Jassby and Platt has been rewritten to make sugar as the end product of photosynthesis (Eq. (4)). In Eq. (1), the parameter alpha (α) describes the initial slope of the curve which levels off to the maximal specific sugar production ($q_{s,m}$). Please note that α can also be expressed as the product of the sugar yield on photons and the specific light absorption coefficient (Eq. (2)) which is in accordance with the approach of Geider [16]. Eq. (3) depicts the relation to calculate the specific photon absorption rate based on the light intensity and the specific light absorption coefficient. By incorporating Eqs. (2) and (3) into Eq. (1), the sugar production rate (Eq. (4)) becomes a function of the maximal specific sugar production ($q_{s,m}$), the specific photon absorption rate (q_{ph}), and the sugar yield on photons ($Y_{s/ph}$) which are process parameters or measurable characteristics of the microalgae. Variable q_{ph} thus replaces I_{ph} in the Jassby & Platt model, and this is practical for the integration of the light model within the growth model, which will be discussed later.

$$q_s = q_{s,m} \cdot \tanh\left(\frac{\alpha \cdot I_{ph}}{q_{s,m}}\right) \tag{1}$$

$$\alpha = Y_{s/ph} \cdot a_x \tag{2}$$

$$q_{ph} = I_{ph} \cdot a_x \tag{3}$$

$$q_s = q_{s,m} \cdot \tanh\left(\frac{q_{ph} \cdot Y_{s/ph}}{q_{s,m}}\right) \tag{4}$$

2.1.2. Aerobic chemoheterotrophic growth model

The sugar produced in the light reaction is exploited as a fundament for new biomass and is oxidized in the mitochondria to obtain extra energy that is necessary to support growth related processes and cell maintenance. This partitioning of sugar between anabolic and catabolic reactions can be described using Pirt's Law (Eq. (5)) [8] which states that a small amount of substrate (sugar) is continuously consumed for maintenance (m_s). The remaining sugar is available for growth (μ) resulting in new biomass according to a constant biomass yield on sugar ($Y_{x/s}$), which indirectly implies that a fixed amount of sugar is respired per carbon mol-x (cmol-x) produced. The validity of adopting Pirt's description for partitioning of photosynthetically derived energy has been established for several microalgae species [17,18]. Please note that the specific sugar production rate (q_s) in Eq. (5) is predicted employing Eq. (4). To summarize, a typical photosynthesis model is combined with the classical aerobic chemoheterotrophic growth model of Pirt to predict the specific growth rate of microalgae (Eq. (5)).

$$\mu_{pre} = (q_s - m_s) \cdot Y_{x/s} \tag{5}$$

2.2. The light attenuation model

Light attenuation within a microalgae suspension in flat plate photobioreactors is described based on the Lambert–Beer Law which states that the attenuation of light over distance is proportional to the light intensity itself with the proportionality constant being the volumetric absorption coefficient. The latter is the product of the specific light absorption coefficient (a_x) and the biomass concentration (C_x).

$$\frac{dI_{ph}}{dz} = -a_x \cdot C_x \cdot I_{ph} \tag{6}$$

The Lambert–Beer Law (Eq. (6)) can be rewritten to extract the specific photon absorption rate (q_{ph}) of microalgae:

$$\frac{\frac{dI_{ph}}{dz}}{C_x} = q_{ph} = -a_x \cdot I_{ph} \tag{7}$$

Taking the integral of the Lambert–Beer from 0 to z results in:

$$I_{ph}(z) = I_{ph}(0) \cdot e^{(-a_x \cdot C_x \cdot z)} \tag{8}$$

and taking into account wavelength dependency the following expression is obtained:

$$I_{ph}(z) = \sum_{\lambda=700}^{\lambda=400} I_{ph,\lambda}(0) \cdot e^{(-a_{x,\lambda} \cdot C_x \cdot z)} \cdot \Delta\lambda \tag{9}$$

By employing Eq. (9) we calculate the light decrease per wavelength, and as such we take into account that green light penetrates deeper compared to red and blue light. The calculation of wavelength dependent incident light intensity ($I_{ph,\lambda}(0)$) is explained in Supplementary files 1. A and 2 which also provides additional detailed information on the wavelength dependency of the specific absorption coefficient. As discussed, we propose the use of the specific photon absorption rate (q_{ph}) within the photosynthesis model. Based on a microbalance of light, we can calculate a local specific photon absorption rate $q_{ph}(z)$ as follows:

$$q_{ph}(z) = \frac{I_{ph}(z) - I_{ph}(z + dz)}{C_x \cdot dz} \tag{10}$$

The variable $I_{ph}(z)$ is then calculated based on Eq. (9).