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# A comparative study of photosynthetic unit models for algal growth rate and fluorescence prediction under light/dark cycles

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ABSTRACT

Accurate description of light-limited algal growth, especially under short light/dark (L/D) cycles, is crucial for prediction of photobioreactor performance and for optimization of operating conditions. Here, a variety of widely used photosynthetic unit (PSU)-based models are evaluated to determine their ability to predict algal specific growth rate and photochemical efficiency under a range of light/dark cycle conditions. Six models were fit to previously published experimental data for algal specific growth rate and photochemical efficiency. Subsequently the weighted sum of squared error (SSE) values, normalized sensitivities to parameter change, and corrected Akaike Information Criterion (AICc) scores were compared. The quality of the fits and the model sensitivities were used to evaluate the assumptions and relative merits of the models considered. For the available data under light/dark cycling conditions, the Bernardi Model scored significantly better on the AICc measure and shows good potential for future use in predicting algal behavior under L/D cycles.

## 1. Introduction

Accurate simulation of algal growth rate is of great importance for reactor design, optimization, and scale-up. In dense cultures typical of those found in photobioreactors, sharp light gradients between illuminated surfaces and dark interior volume exist. Several studies have demonstrated that low frequency transitions of microorganisms between these light and dark zones ($< 0.01$ Hz) do not increase algal productivity [1,2], but that under high frequency light/dark cycles the efficiency of light usage improves and growth rate can increase substantially [3]. This mixing-induced light/dark cycle effect can be exploited by designing photobioreactors so that they produce flow structures capable of rapidly shuttling microorganisms between light and dark regions of the reactor [4,5]. Hence, in order to optimize the design and operation of algal photobioreactors, it is essential to be able to accurately predict algal growth rate under a wide range of light/dark (L/D) cycle conditions.

More than 40 algal productivity models have been published [6] in recent years. Among these, dynamic mechanistic models based on the concept of reaction centers comprising photosynthetic units (PSUs) are capable of accounting for short L/D cycles and are amenable for use in engineering models. Because these models assume that all photosynthetic processes take place in PSUs, the result is a dramatic but practical simplification of the complex processes involved in photosynthesis [7]. In PSU-based models, at any moment each PSU in a cell is assumed to be in one of a limited number of states including resting, activated, or inhibited. Various possible transitions between these states can be considered, such as the activation of resting PSUs upon receiving sufficient photosynthetic radiation or the inhibition of active PSUs upon overexposure to light, which disables photosynthetic capabilities. The productivity and growth rate of cells are generally assumed to be directly related to the flux of PSUs from the active to the resting state, which represents photochemical quenching, in which energy is passed on to the respiratory processes of the cell. Similarly, the fraction of inhibited PSUs is associated with algal fluorescence characteristics.

Although several PSU-based models are available, no comprehensive comparison of the performance of widely used variants is currently available. Without such a model comparison, it is difficult to determine which of the various sets of assumptions leads to the most accurate predictions. The variety of measurements used to fit models in previous studies also makes direct comparisons difficult. To resolve these issues, we consider several specific PSU models and compare their predictions for specific growth rate and fluorescence using a common experimental data set. As a result of this analysis, it should be possible to make better-informed model choices for simulation of algal growth rate and fluorescence in a photobioreactor undergoing L/D cycles.

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The paper is organized as follows. First, model assumptions and equations are reviewed, and analytical or numerical solutions for specific growth rate and photochemical efficiency under L/D cycle conditions are developed. Second, the methods for fitting each of the models to experimental data are described. Third, the results of the model fits and the parameter estimates are reported. Fourth, the results of a sensitivity analysis for each model are considered. Finally, the relative merits of the various models considered are discussed.

## 2. PSU model equations

The predictions for time-averaged specific growth rate ($\overline{\mu}$) and photochemical efficiency ($\overline{q}$) from six distinct PSU models were computed under the assumption that algal cultivation occurs under L/D cycles. These cycles are assumed to consist of a light exposure period of duration $t_l$ wherein microorganisms are irradiated at a constant photon flux $I$ followed by a sudden transition to a “dark” period of duration $t_c$ - $t_l$ wherein microorganisms receive no photosynthetic radiation. Hence, the period for a single cycle is $t_c$. For the three-state models considered, the fractions of total PSUs that reside in the resting, active, and inhibited states are given by $x_1$, $x_2$, and $x_3$ respectively, and hence $\Sigma x_i = 1$. We also consider a four-state model [8] that includes two distinct active states. Some models account for variable total number or concentration of PSUs, and in these cases $a_i$ refers to the number or concentration of PSUs in state $i$, so that $\Sigma a_i = a_t$. In the following analyses, it was also assumed that cells were photoacclimated at light intensity $I$ (equal to the intensity occurring during the irradiation period of an L/D cycle) and had reached a quasi-steady state in which $x_i(0) = x_i(t_c)$ for all $x_i$. Schemes depicting state transitions for the six PSU models considered here are shown in Fig. 1.

### 2.1. Wu model

The Wu model [9] is a modified version of the Eilers and Peeters model [14] and it assumes that fluxes of PSUs from $x_1$ to $x_2$ (resting to active) and $x_2$ to $x_3$ (active to inhibited) are first-order with respect to light intensity. In contrast, fluxes of PSUs from $x_3$ to $x_1$ (inhibited to resting) and $x_2$ to $x_1$ (active to resting) are independent of light intensity. These assumptions lead to the following set of differential equations.

$$\frac{dx_1}{dt} = -\alpha I x_1 + \gamma x_2 + \delta x_3 \tag{1a}$$

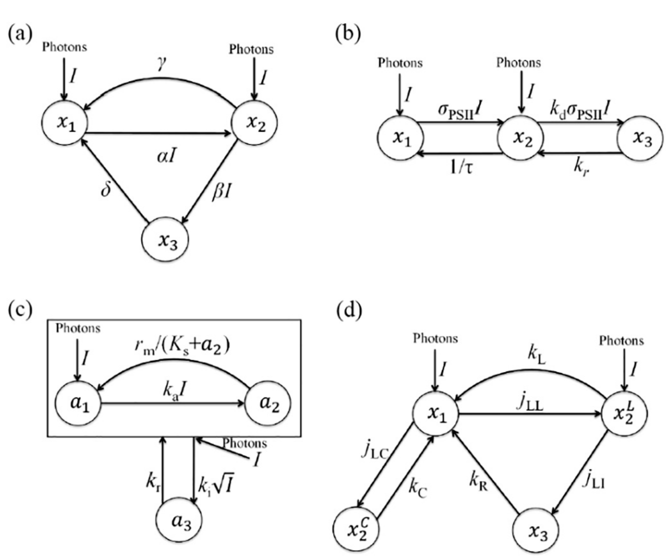


**Fig. 1.** (a) Wu model [9]. (b) Han model [10]. The Nikolaou model [11] has a similar scheme. (c) Camacho-Rubio model [12]. The Bernardi model [13] has a similar scheme. (d) Papadakis model [8].

$$\frac{dx_2}{dt} = \alpha I x_1 - \beta I x_2 - \gamma x_2 \tag{1b}$$

$$\frac{dx_3}{dt} = \beta I x_2 - \delta x_3 \tag{1c}$$

The instantaneous specific growth rate $\mu$ is computed from a term proportional to the flux of PSUs from the activated to the resting state minus a constant maintenance term represented by $Me$, as shown in Eq. (2a). The ratio of variable fluorescence to maximum fluorescence, also known as photochemical efficiency ($F_v/F_m$ or $q$), was assumed to be first-order with respect to the fraction of non-inhibited PSUs as in Eq. (2b).

$$\mu = k\gamma x_2 - Me \tag{2a}$$

$$q = f'(1 - x_3) \tag{2b}$$

The derivation of analytical solutions for $x_1(t)$ and $x_2(t)$ over an L/D cycle has already been reported by Wu and Merchuk [9]. Using these solutions, the mean values for specific growth rate and photochemical efficiency over an L/D cycle are given by:

$$\overline{\mu} = \frac{k\gamma}{t_c}\int_0^{t_c} x_2(t)dt - Me \tag{3a}$$

$$\overline{q} = \frac{f'}{t_c}\int_0^{t_c} [x_1(t) + x_2(t)]dt \tag{3b}$$

The seven adjustable model parameters include $\alpha$, $\beta$, $\delta$, $\lambda$, $k$, $Me$, and $f$.

### 2.2. Han model

The Han model [10] assumes that PSU fluxes from $x_1$ to $x_2$ (activation) and from $x_2$ to $x_3$ (inhibition) are first-order with respect to the irradiance and the effective absorption cross-section of PSII ($\sigma_{PSII}$). In this model, repair of PSUs is modeled by flux from $x_3$ to $x_2$, which is assumed to be zero-order with respect to irradiance. Flux from $x_2$ to $x_1$ (deactivation) is assumed to be first-order with respect to the inverse of the time constant $\tau$, which represents the turnover time of the electron transfer chain. These assumptions lead to the following equations:

$$\frac{dx_1}{dt} = -I\sigma_{PSII}x_1 + \frac{x_2}{\tau} \tag{4a}$$

$$\frac{dx_2}{dt} = I\sigma_{PSII}x_1 - \frac{x_2}{\tau} + k_r x_3 - k_d I\sigma_{PSII}x_2 \tag{4b}$$

$$\frac{dx_3}{dt} = -k_r x_3 + k_d I\sigma_{PSII}x_2 \tag{4c}$$

A quasi-steady-state solution under L/D cycles can be derived for this model by considering the light and dark portions of the L/D cycle separately and by enforcing periodic boundary conditions, leading to analytical solutions for the light and dark periods:

$$x_{2,light} = C_1 e^{C_1^H t} + C_2 e^{C_2^H t} + \frac{C_5^H}{C_4^H} \tag{5a}$$

$$x_{1,light} = \frac{C_6^H C_1 e^{C_1^H t} + C_7^H C_2 e^{C_2^H t} + C_8^H \frac{C_5^H}{C_4^H} - k_r}{I\sigma - k_r} \tag{5b}$$

$$x_{2,dark} = C_3 e^{-\frac{t}{\tau}} + C_4 e^{-k_r t} \tag{6a}$$

$$x_{1,dark} = -C_3 e^{-\frac{t}{\tau}} - \frac{C_4 e^{-k_r t}}{k_r \tau} + 1 \tag{6b}$$

Definitions of constants are as follows: $C_1^H = -\frac{C_3^H + \sqrt{C_3^{H2} - 4\tau C_4^H}}{2\tau}$, $C_2^H = -\frac{C_3^H - \sqrt{C_3^{H2} - 4\tau C_4^H}}{2\tau}$,