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An Algae-Growth CFD Model Including the Effects of CO_2 Concentration and pH

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Abstract

Microalgae are a promising source of biofuels but production costs remain high. Models are relatively inexpensive tools that can be used to enhance economic competitiveness through system and operation optimization that minimizes energy and resource (e.g., CO_2) consumption and maximizes algal oil yield.

Inorganic carbon in water is available as free dissolved CO_2, carbonic acid (H_2CO_3), bicarbonates (HCO_3^-), and as carbonates (CO_3^{2-}). For photosynthesis, most algae species use dissolved CO_2. pH is a function of the chemical equilibrium between the different forms of inorganic carbon and a high pH indicates less availability of free dissolved CO_2. Hence, pH of the medium affects algae photosynthesis, their growth, and oil production rates. There is a fine line between too little CO_2 starving algae growth and too much yielding an acidic medium that inhibits growth; its addition to the system should be optimized.

Sandia has developed a model (SNL-EFDC) that uses modified versions of the US EPA's Environmental Fluid Dynamics Code (EFDC)[1] in conjunction with the US Army Corp of Engineers' water-quality code, CE-QUAL[2], to couple hydrodynamics and atmospheric-driven thermodynamics to algae-growth kinetics. The model allows manipulating variables associated with nutrient availability, temperature, light intensity and pH. Model results demonstrate that growth is appropriately inhibited when pH and CO2 limitations were added. Simulations can identify optimal CO_2 concentrations that maximize growth of a specific algae strain.

Growth Model

$$\frac{\partial B}{\partial t} = (P - B_M - P_R)B + \frac{\partial}{\partial z}(w_s B) + \frac{B_L}{V}$$

Governing equation for algae growth

B (g/m^3) - biomass, t (days) - time, P (day^{-1}) - production (growth) rate, B_M (day^{-1}) - basal metabolic rate, P_R (day^{-1}) - predation rate, w_s (m/day) - settling velocity, B_L (g/day) - external loads such as deposition or sources, V (m^3) - model cell volume

$$P = P_M f(n) g(I) h(T) i(\mathrm{pH})$$

Decoupled growth equation

P_M (day^{-1}) - maximum production rate under optimal conditions, $f(v)$ - effect of non-optimal nutrients (includes CO_2 limitation) ($0 \le f(v) \le 1$), $g(I)$ - effect of non-optimal illumination ($0 \le g(I) \le 1$), $h(T)$ - effect of non-optimal temperature ($0 \le h(T) \le 1$), and i(pH) - effect of non-optimal pH ($0 \le i(\mathrm{pH}) \le 1$).

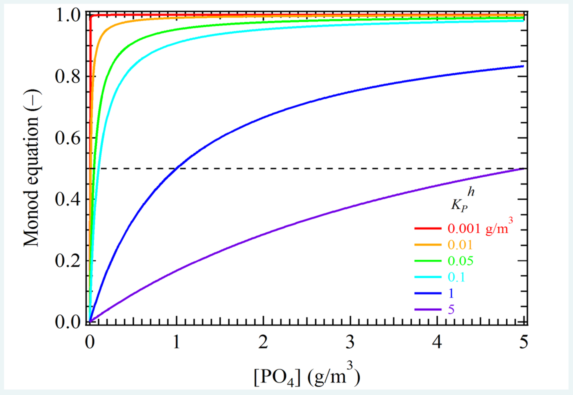

Figure 1: Limiting nutrient availability for phosphate

Monod equation for nutrient availability

$$f(n) = \frac{n}{K_P^h + n}$$

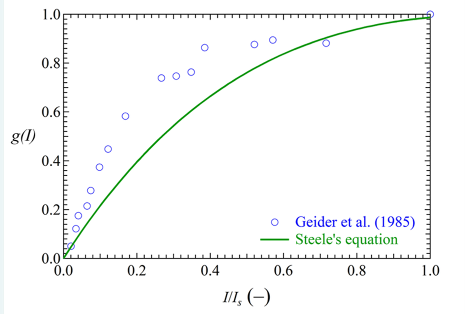

Figure 2: Limitation due to non-optimal illumination

Steele's equation for light limitation[4]

$$g(I) = \frac{I(z)}{I_s}\exp\left(1 - \frac{I(z)}{I_s}\right)$$

Riley's light extinction[5]

$$K_e = k_B + 0.0088B + 0.054B^{2/3}$$

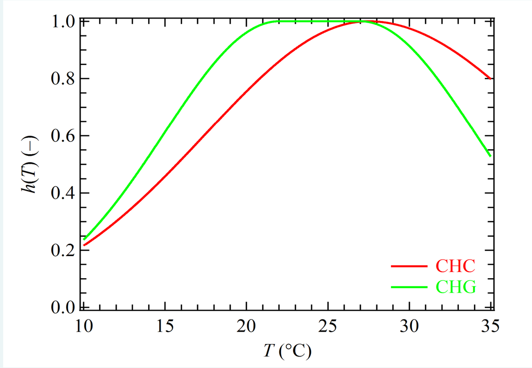

Figure 3: Limitation due to non-optimal temperature [6]

$$h(T) = \begin{cases} \exp\left[-KTG_{1x}(T - TM_{1x})^2\right] & \text{for } T \le TM_{1x} \\ 1 & \text{for } TM_{1x} \le T \le TM_{2x} \\ \exp\left[-KTG_{2x}(TM_{2x} - T)^2\right] & \text{for } T > TM_{2x} \end{cases}$$

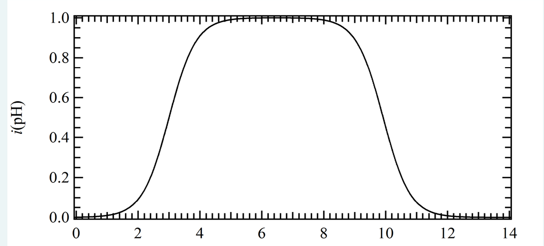

Figure 4: Limitation due to non-optimal pH [7]

$$[H^+] = 10^{(-\mathrm{pH})}$$

$$i([H^+]) = \frac{[H^+]}{[H^+] + k_{OH}(T) + [H^+]^2/k_H(T)}$$

$$\mathrm{pH} = -\frac{1}{2}\log_{10}(k_w + k_1 k_h [CO_2])$$

Verification and Validation

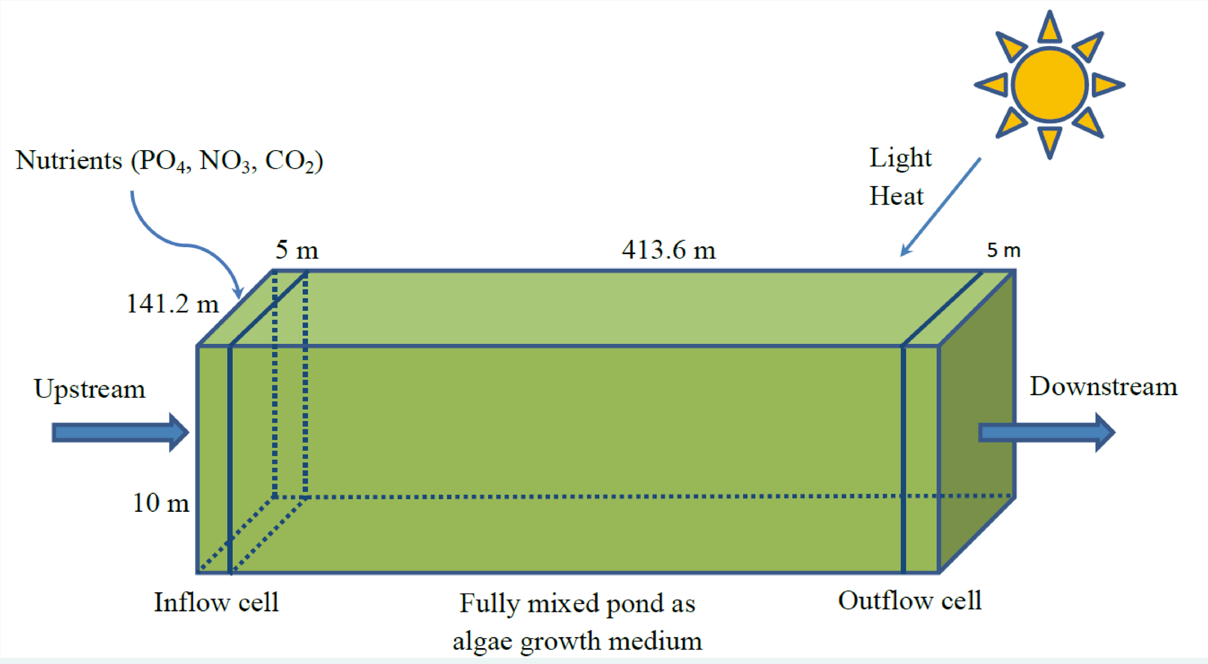

Figure 5: Schematic of the pond used to model example problem 33-2 from Chapra's *Surface Water Quality Modeling* [8]

- Center cell is a single-layer fully mixed lake (413.6 m long, 141.2 m wide, 10 m deep). Boundary conditions are defined on inflow and outflow cells (5 m long , 141.2 m wide, 10 m deep).
- Input flow provides algae (0.033 g/m^3), phosphorus (0.01 g/m^3), and water (0.0772 m^3/s).
- Output flow removes fully mixed constituents at the rate of 0.0772 m^3/s.

Table 1: System parameters for Chapra's example and Greenhouse model

Parameters	Chapra example 33-2	Greenhouse model
Initial concentration of chlorophyll/algae	0.5 mg Chl-a/m^3	40.6278 g/m^3
Maximum growth rate under optimal conditions	1 /day	4.25 /day
Loss due to combined respiration and excretion	0.1 /day	0.1 /day
Predation rate	0 /day	0 /day
Initial phosphorus concentration	9.5 mg P/m^3	3.1 g P/m^3
Input flux of phosphorus concentration	10 mg P/m^3	0 mg P/m^2
Half-saturation constant for phosphorus	2 mg P/m^3	2 mg P/m^3
Initial nitrate concentration	In excess	54.72 g/m^3
C:N ratio	6	25.3
C:P ratio	43.3	430
Initial CO_2 concentration	NA	0.902 g/m^3
Half-saturation constant for CO_2	NA	0.02772 g/m^3 [9]
Average light over daylight hours	400 ly/day	Variable
Background light extinction	0.1 /m	0.45 /m [10]
Optimal light intensity	250 ly/day	173 ly/day [11]
Photo period (fraction of day)	0.5	Variable
Minimum optimal temperature	20°C	18°C
Minimum suboptimum temperature effect coefficient	0 °C^{-2}	0.69°C^{-2}
Maximum optimal temperature	20°C	22°C
Maximum suboptimum temperature effect coefficient	0 °C^{-2}	0.007°C^{-2}
Water depth	10 m	0.211 m
-No benthic flux. -Constant reaeration. -No wind forcing. -No settling velocity.. -Riley's total light extinction.		

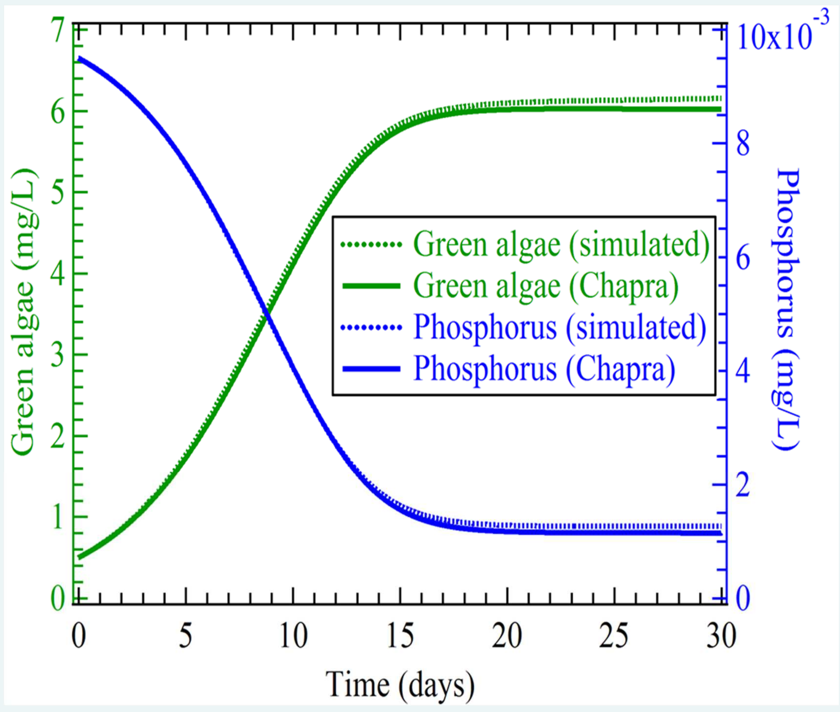

Figure 5: Validation of algae growth model with Chapra's example

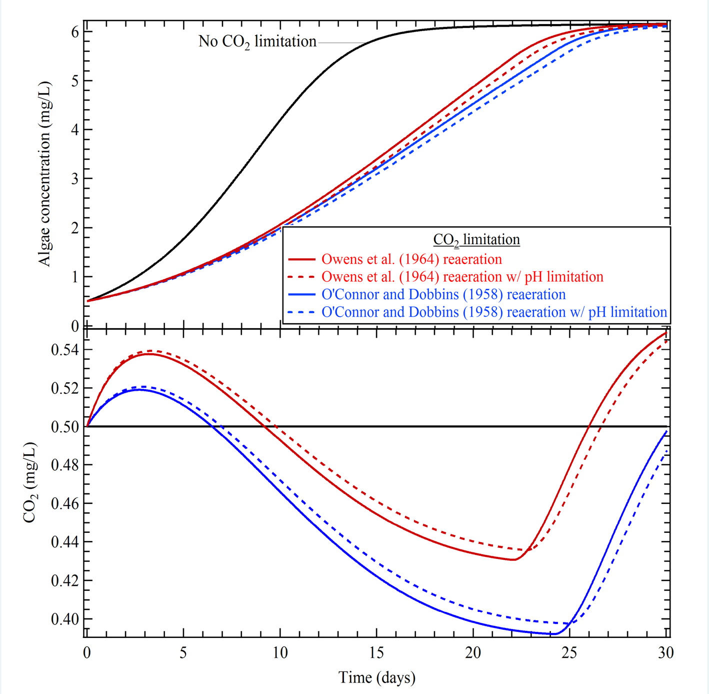

Figure 6: Chapra's example 33-2 with CO_2 and pH limitations

- Figure 5 shows excellent agreement between Chapra's analytical solution and SNL-EFDC simulations for algae and total phosphorus concentration.
- Figure 6 shows simulations results without (solid curves) and with (dashed curves) pH limitation using one of two options for reaeration.
- In reaeration models, initially CO_2 concentrations increase due to reaeration while algae concentrations are quite low. As biomass increases, CO_2 concentrations decrease accordingly.
- As the algae growth rate decreases to zero, CO_2 levels increase due to reaeration supplying sufficient CO_2 to sustain the algae population at a constant concentration.
- In addition to CO_2 limitation, by including pH limitation, growth is further decreased.

Greenhouse model

- This model simulates growth of *Nannochloropsis salina* in a real pond maintained inside a greenhouse under known temperature and irradiance conditions.
- Schematics of the model is similar to the schematic shown in Figure 5 except that there are no nutrients added to the system other than CO_2 and there is no flow. A high C:N:P ratio of 430:17:1 (to simulate a nonideal nutrient environment) is assumed.
- Pond dimensions: 1.666 m long, 1.5 m wide, 0.211 m deep containing 0.53 m^3 of growth medium.
- After 52 days, algal growth was inhibited by adding acid to the pond (no fit sought thereafter).
- Other model parameters are listed in Table 1 (notably B_M= 0.1 /day and half-saturation constants).

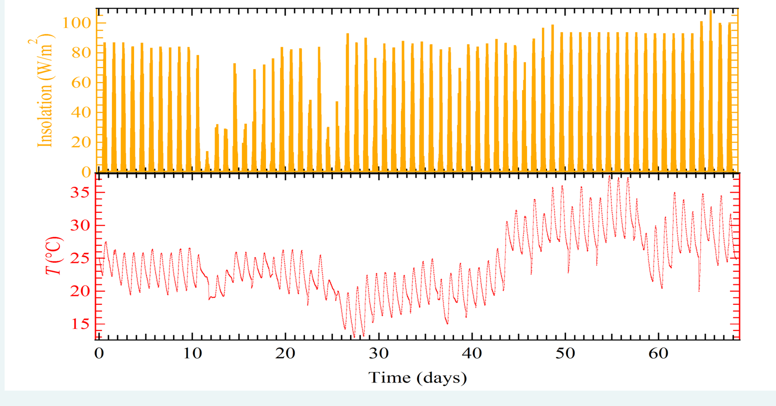

Figure 7: Light exposure and temperature of the algae pond

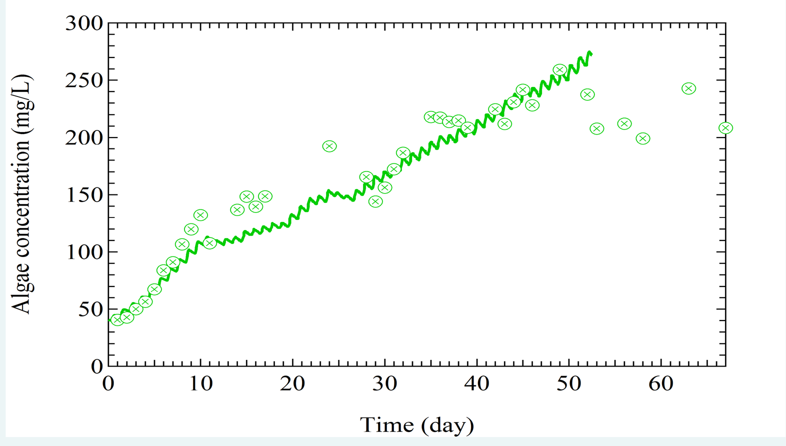

Figure 8: Algal biomass from the greenhouse experiment and corresponding model

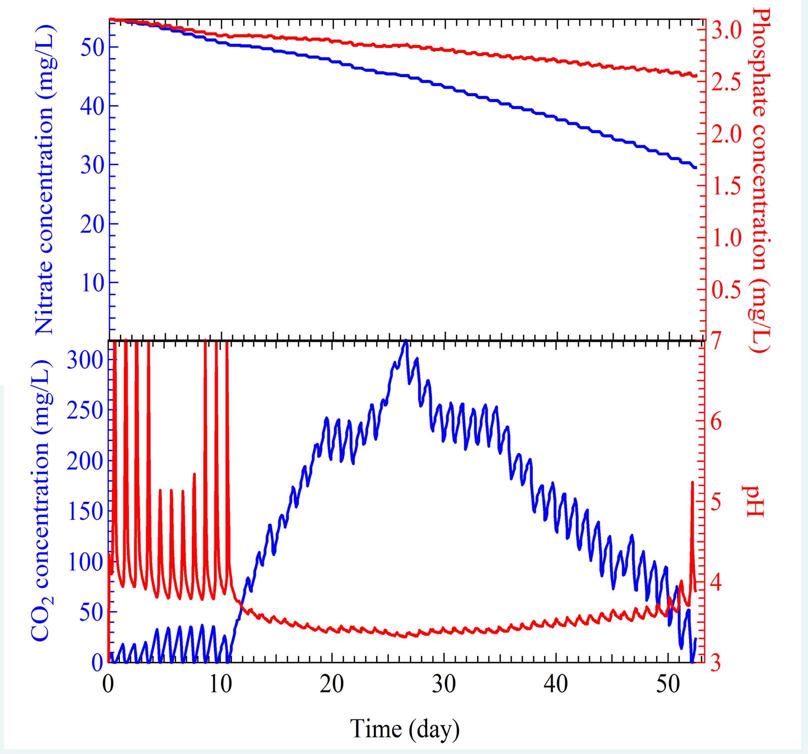

Figure 9: Nutrients, CO_2 and pH for the greenhouse simulation

Maximum growth rate for the model was obtained by performing a least squares fit of algal biomass growth to match measured concentrations using a parameter estimation code, PEST[12]. A maximum growth rates of 4.25 /day was estimated for C:N:P = 430:17:1 and B_M = 0.1 /day.

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