Formation of Algae Growth and Lipid Production Constitutive Relations for Improved Algae Modeling

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LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Early Career R&D Program

Sandia National Laboratories

PI: Patricia E. Gharagozloo (8365), Mentor: Todd W. Lane (8263)

Problem

Why Algae?

- Algae-based biofuels are a promising component to a long-term renewable energy solution
- Algae can be engineered or stressed to produce large quantities of oil with favorable characteristics for biodiesel
- Algae can be grown in waste/brackish/sea water, reducing the impact on fresh water supplies
- Algae mitigate atmospheric CO_2
- Algae can be grown on non-arable land, decreasing the impact on the food supply
- Algae growth and harvesting still require much optimization to reduce the cost of oil production and improve efficiency

- How can we easily optimize algae growth and lipid production for different environmental conditions?
- What bioreactor designs yield the best growth efficiencies?
- What types of algae works best a different times of years or different locations?

We need a realistic model

- We need to be able to optimize algae growth and lipid production in large commercial scale systems
- It is too time consuming and expensive to test various solutions on a commercial scale
- A computational model facilitates faster and cheaper optimization
- The necessary data are lacking to create the needed constitutive relations for algae growth and lipid production.

Approach

Multi-factorial Measurements

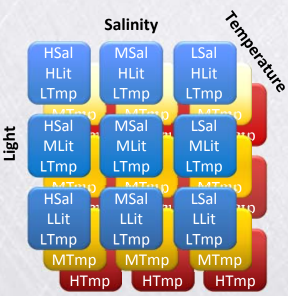
- Measure effect of light intensity, temperature and salinity on growth multiple key marine algal species
- Use in-situ measurement methods and parallel growth to reduce time needed

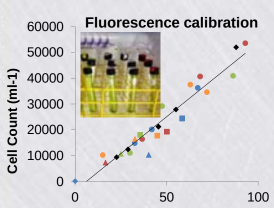
Constitutive Relations

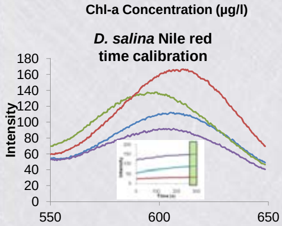
- Determine relationships between environmental variables and growth
- Apply to algae growth model

Photobioreactor Models

- Develop model for closed photobioreactor systems
- Expand model to use of marine algal species
- Add lipid production to model







Measurement Techniques

- Algae Selection:
  - Marine, triacylglycerol (TAG) producing, readily available
  - *Dunaliella salina, Chlorella sorokiniana, Nannochloropsis oculata, Nitzschia frustulum*
- Factors:
  - Sample 4 salinities, 3 light intensities, 3 temperatures
- Growth:
  - Measure chlorophyll a fluorescence
  - Excite at ~440 nm, emit at ~670 nm
  - Calibrate chlorophyll fluorescence with known standards of chlorophyll concentration
  - Calibrate chlorophyll concentration with cell counter for each algae species
- Lipids:
  - Use Nile-red-stained lipid fluorescence
  - Excite at ~530 nm, emit at ~600 nm
  - Calibrate for cell penetration time period for each algae species
  - Calibrate intensity with extraction analysis for each algae species

EFDC and Water Quality Model

- Modified version of the Environmental Protection Agency's Environmental Fluid Dynamics code and U. S. Army Corp of Engineer's water-quality model.
- Models algae growth based on constitutive relations

B – biomass concentration (gC/m³)
P – production rate (1/d)
B_M – metabolism rate (1/d)
P_R – predation rate (1/d)
f – growth limiting constitutive relations

$$\frac{\partial}{\partial t}B(\mathbf{x},t)=(P-B_M-P_R)B(\mathbf{x},t)$$
$$P=\mu_{opt}\cdot\left[f_1(N)f_2(I)f_3(T)f_5(S)\right]$$

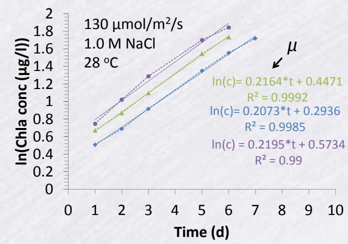
- Tracks nutrients, salinity, temperature, light, CO_2 and O_2 concentrations
- Allows for sources and sinks of parameters

Results

Growth Measurements

- Measured growth at 28, 31, and 33 °C for 3 light intensities and 4 salinities in parallel
- Bubble air into samples
- Light/dark cycle = 16:8
- Measured in triplicate and averaged
- Calculate specific growth rate, μ, by fitting data to exponential growth curve:

$$C_{Chla}=C_0\,e^{\mu t}$$
$$\ln(C_{Chla})=\mu t+\ln(C_0)$$



Constitutive Relation Determination

Salinity:

- Bell curve, above and below optimum decay coefficients, non-zero asymptote

$ksal_1$ = 0.0001 (ppt NaCl)$^{-2}$
$ksal_2$ = 0.0003 (ppt NaCl)$^{-2}$
S_{opt} = 59 ppt NaCl (1.01 M)
f_{sal} = 0.6

$$f(S)=\frac{\mu(S)}{\mu_{opt}}=\begin{cases}\left(f_{sal}\exp\left(-ksal_1\left(S-S_{opt}\right)^2\right)+\left(1-f_{sal}\right)\right) & when\ S\le S_{opt}\\ \left(f_{sal}\exp\left(-ksal_2\left(S-S_{opt}\right)^2\right)+\left(1-f_{sal}\right)\right) & when\ S>S_{opt}\end{cases}$$

Light Intensity:

- Use Steele's equation for light intensity constitutive relation

I_{opt} = 150 μmol/m²/s
FD = ⅔ (from 16:8 light/dark cycle)

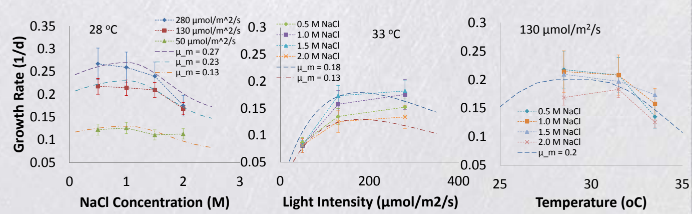
$$f(I_0)=\frac{\mu(I_0)}{\mu_{opt}}=\frac{2.718\cdot FD}{Kess\cdot\Delta z}\left(e^{-\alpha_B}-e^{-\alpha_T}\right)$$
$$\alpha_B=\frac{I_0}{FD\cdot I_{opt}}e^{-Kess(H_T+\Delta z)},\quad \alpha_T=\frac{I_0}{FD\cdot I_{opt}}e^{-Kess\cdot H_T}$$
$$Kess=Ke_b+Ke_{Chl}\frac{B}{CChl}$$

Temperature:

- Gaussian curve, above and below optimum decay coefficients

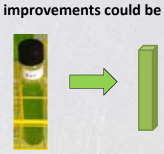
k_{T1} = 0.03 (°C)$^{-2}$
k_{T2} = 0.025 (°C)$^{-2}$
$T_{opt,1}$ = 28 °C
$T_{opt,2}$ = 30 °C

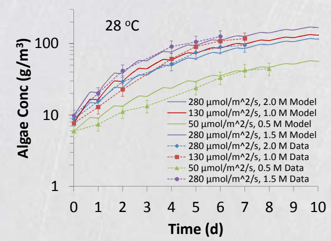
$$f(T)=\frac{\mu(T)}{\mu_{opt}}=\begin{cases}\exp\left(-k_{T1}\left(T-T_{opt,1}\right)^2\right) & T\le T_{opt,1}\\ 1 & T_{opt,1}<T\le T_{opt,2}\\ \exp\left(-k_{T2}\left(T-T_{opt,2}\right)^2\right) & T>T_{opt,2}\end{cases}$$



Lab-scale Model and Data Comparison

- Predicted *D. salina* growth in test tube based on constitutive relations (measurement (*S,I,T*) and literature (*N*))
- Relations chosen work relatively well, more improvements could be made





Significance

The knowledge gained will enable computational models to optimize algae growth in real-world conditions with varying temperature, light, and salinity over the course of a day or year.

Through a validated constitutive growth model, algae performance and production efficiency can be predicted for various growth conditions, including different weather climates and reactor designs. The model will enable improved design and algae strain selections.

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