# Modeling HABS with CE-QUAL-W2: Approaches and Future Challenges

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# Cyanobacteria – Attributes

- Single celled, photosynthetic organisms with high reproduction rates
- Some cyanobacteria
	- Control their buoyancy and thus vertical position in the water column
	- Fix atmospheric nitrogen (N2)
	- Produce toxins (e.g., neurotoxins, hepatotoxins)
	- Form colonies that aid with mobility, reduced predation, and shade out competition
	- Have unique reproductive strategies
	- Other unique attributes.
- Harmful algal blooms (HABS) are typically related to blooms that include toxin producing strains, create public health hazards and/or environmental impacts
- Nuisance blooms of non-toxic species also occur

#### CE-QUAL-W2

- Two-dimensional laterally averaged model
- Hydrodynamic and water quality model
- Capable of modeling a wide suite of water quality constituents including detailed representation of multiple algae groups
- **ALPO** Chl a to algal biomass conversion factor, phytoplankton, mg Chl a to mg-A ALP1 Fraction of algal biomass that is nitrogen, phytoplankton, mg-N/mg A Fraction of algal biomass that is phosphorous, phytoplankton, mg-P/mg A ALP<sub>2</sub> MUMAX Maximum specific growth rate, phytoplankton, 1/d **RESP** Local respiration algae, phytoplankton, 1/d **RESP** Local mortality rate of algae, phytoplankton, 1/d  $SIG1$ Settling rate of algae, phytoplankton, 1/d Half saturation coefficient for light, phytoplankton, KJ m-2 s-1 **KLIGHT PREFN** Preference factor for NH3-N, phytoplankton **ABLPO** Chl a to algal biomass conversion factor, bed algae, mg Chl a to mg-A BMUMAXMaximum specific growth rate, bed algae, 1/d Local respiration rate of algae, bed algae, 1/d **BRESP GRAZE** Local respiration rate of algae, bed algae, 1/d Local respiration rate of algae, bed algae, 1/d **BMORT** KBLIGHT Half-saturation coefficient for light, bed algae, KJ m-2 s-1
- **KBLIGHT Half-saturation coefficier** PBREFN Preference factor for NH3 BET1 Rate constant: biological BET2 Rate constant: biological BET3 Rate constant: hydrolysis **KNINH** First order nitrification in  $K1$ Deoxygenation rate const Minimum reaeration rate Michaelis-Menton half sa **KNITR KPHOS** Michaelis-Menton half sa Fraction of algal biomass ABLP1 ABLP2 Fraction of algal biomass Half-saturation coefficier **KBNITR**



# Case Studies

#### • CE-QUAL-W2 Modeling Approaches - Processes

- Representing buoyancy compensating cyanobacteria
- Representing nitrogen fixing cyanobacteria
- Representing dissolved oxygen constraints on growth and mortality\*
- CE-QUAL-W2 Modeling Approaches Prescriptions
	- Enhanced mixing (cove)
	- Barrier Curtain\*
	- Algaecide Treatment\*
	- Reservoir Drawdown\*
	- Hypolimnetic oxygenation\*

\* Not covered herein

# CE-QUAL-W2 Phytoplankton Logic

- Complex representation
- Multiple algae groups
- Other water quality interactions
- Temperature dependent





where:

- $z =$  cell height
- $Z_u$  = net growth rate of a zooplankton species
- $\sigma$  = zooplankton grazing preference factors

$$
\zeta_{ag} = \text{algal growth rate}, \text{sec}^1
$$

- $K_{ar}$  = algal dark respiration rate, sec<sup>-1</sup>
- $K_{ae}$  = algal excretion rate, sec<sup>-1</sup>  $K_{\text{am}} =$  algal mortality rate, sec<sup>-1</sup>
- $\omega_a$  = algal settling rate, *m* sec<sup>-1</sup>
- $\Phi_a$  = algal concentration, g m<sup>-3</sup>

# CE-QUAL-W2 Phytoplankton Logic

- Complex representation
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 $\partial \varPhi_a$  $S_a = K_{ag} \Phi_a - K_{ar} \Phi_a - K_{ae} \Phi_a - K_{am} \Phi_a$  $\partial \overline{z}$ respiration excretion mortality settling  $-\sum_{\alpha=1}^{\infty}\left(Z_{\mu}\varPhi_{\alpha\alpha} \frac{\sigma_{\alpha_{1g}}\varPhi_{\alpha}}{\sum\sigma_{\alpha_{1g}}\varPhi_{\alpha}+\sigma_{\rho o m}\varPhi_{\rho o m}+\sum\sigma_{\alpha o}\varPhi_{\alpha o}}\right)$ net loss to grazing

where:

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- 
- $\omega_a$  = algal settling rate, *m* sec<sup>-1</sup>
- $\Phi_a$  = algal concentration, g m<sup>-3</sup>

# Vertical Movement of Cyanobacteria

- Gas Vesicles are used to "control" location in water column (formation, collapse, protein or carbohydrate content, environmental conditions, colony size/structure, other)
- Preferential position
	- Light
	- Nutrients
	- Competition
- Complex process



#### Settling Rate  $(S_a = f(\omega_a))$  $\partial \Phi_a$  $\frac{\partial \Psi}{\partial z}$ ))

- Positive  $\omega_a$ : negatively buoyant
- Negative or zero  $\omega_a$ : positively buoyant or neutrally buoyant
- Subject to simulated aquatic system mixing processes
- CE-QUAL-W2 Existing Formulation
	- Cyanobacteria or other floating phytoplankton: 0.0-0.05 m day-1 and can specify a negative settling velocity (CE-QUAL-W2 2021)
	- Settling rate = 0 (Smith and Kiesling 2019)
- CE-QUAL-W2 Modified Formulation
	- Use specific logic to model vertical migration (Overman 2019\*) new code
	- Parameterization (field data) challenge

# Nitrogen Fixation Growth  $(S_a = f(K_{ag}\Phi))$

- Limiting growth factor
	- Light
	- Phosphorus
	- Nitrogen
	- Silica
- Heterocyst: specialized fix nitrogen (N2)



 $K_{ag} = \gamma_{ar} \gamma_{af} \lambda_{min} K_{agmax}$ 

where:

- $\gamma_{ar}$  = temperature rate multiplier for rising limb of curve
- $\gamma_{\text{af}}$  = temperature rate multiplier for falling limb of curve
- $\lambda_{min}$  = multiplier for limiting growth factor (minimum of light, phosphorus, silica, and nitro $gen)$
- $K_{ag}$  = algal growth rate, sec<sup>-1</sup>
- $K_{\text{agmax}} = \text{maximum algal growth rate}, \text{sec}^{-1}$



where:

 $\Phi_i$  = phosphorus or nitrate + ammonium concentration, g m<sup>-3</sup>

 $P_i$  = half-saturation coefficient for phosphorus or nitrate + ammonium, g  $m<sup>3</sup>$ 

# Nitrogen Fixation Growth  $(S_a = f(K_{aa} \Phi))$

#### • CE-QUAL-W2 – Existing Formulation

• Set half saturation coefficient for nitrate and ammonia to zero

 $\lambda_i(P_i = 0) =$  $\Phi_i$  $\Phi_i$  $= 1.0$ 

- No nutrient limitation
- Allows
	- Cyanobacteria to reproduce under low inorganic nitrogen concentrations
	- Effectively incorporates "load" due to N-fixation consistent with algae stoichiometry (≈0.08)



## Prescription: Mixing a Cove

- Conceptualized isolating a cove using a barrier curtain
- Used CE-QUAL-W2 to assess mixing required to disrupt cyanobacteria
- Used vertical turbulent diffusion coefficient as a metric after Huisman et al. (2004)





### Mixing Impacts on Microcystis

- Vertical mixing in the water column reduces the advantages of colonization and buoyancy compensation by vacuolated cyanobacteria
- If mixing is sufficient and depth great enough, other species can outcompete cyanobacteria



Predicted response of *Microcystis*, diatoms, and green algae as a function of water-column depth and turbulent diffusion (from Huisman et al. 2004).

## Leveraging CE-QUAL-W2

- Using the temporal and spatial distribution of heat in the cove (eqtn  $(1))...$
- Calculate eddy diffusivity values (eqtn 2) using simulated CE-QUAL-W2 vertical temperature profiles
- Three conditions
	- No curtain
	- Curtain with no circulation
	- Curtain with circulation
- Calculate turbulent diffusion coefficient (eqtn 2) and compare with Huisman



- = maximum water depth (cm)  $Z_{\rm max}$
- = water density [grams per cubic centimeter  $(g/cm^3)$ ] ρ
- $=$  mass [grams (g)] g
- = specific heat of water [Joules per degree Celsius per gram g (J/°C·g)]  $C_{D}$
- T = water temperature [degrees Celsius (°C)]
	- $=$  time [seconds (s)]
- = water body surface area at depth z [square centimeters (cm<sup>2</sup>)]  $F(z)$
- = solar (short-wave) radiation at depth z [watts per square centimeter (W/cm<sup>2</sup>)]  $R(z)$
- = sediment heat exchange [Joules per square centimeter second  $(J/cm^2-s)$ ]  $H(z)$
- $=$  sediment area at depth z (cm<sup>2</sup>)  $I(z)$

Solving for the turbulent diffusion coefficient  $(K<sub>2</sub>(z))$  yields:

$$
(2) \qquad K_z(z) = \left[ - \int_z^{z_{max}} \rho C_p \frac{dT}{dt} F(z) dz + R(z) F(z) - \int_z^{z_{max}} H(z) l(z) dz \right] \cdot \left[ \rho C_p \frac{dT}{dz} F(z) \right]^{-1}
$$

(see Jassby and Powell (1975) and Benoit and Hemond (1974)



# Results

[Deg C]

is-18

 $20 -$ 

 $22 24$ 

 $26$ 

28

**an** 

[Deg C]

 $16 18<sub>1</sub>$ 

 $20 22 24<sub>1</sub>$ 

 $26 -$ 

 $28$ m-

Velocity

 $[$ Deg $C]$ 

Ĩß. 18

20  $\boldsymbol{z}$ 

24

26

28

30

Velocity

 $0.02 \, \mathrm{m/s}$ 

 $0.02$  m/s

- Curtain with 1 cms (35.3 cfs) circulation produces  $K_{1/2}$  from 2 cm<sup>2</sup>/s to >50 cm<sup>2</sup>/s in top 8 m of cove (Secchi 1.0-1.5m)
- Hydraulic residence time <5 days
- Results suggest viable control measure in this 10 m cove



# Cyanobacteria Representation in CE-QUAL-W2: Considerations

- Blooms are often spatially heterogeneous (x-y-z) and dynamic through time
- Grid resolution is a key consideration, depending on objective
- Thermal stratification -> effectively modeled
- Water quality dynamics -> effectively modeled
- Species/group competition is challenging
- Can require considerable field observations to parameterize and test model for cyanobacteria simulation
- Recommend starting big (seasonal responses) and refine as needed

# Discussion

## Citations

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- Overman, Corina Christina Mae, "Modeling Vertical Migration of Cyanobacteria and Zooplankton" (2019). Dissertations and Theses. Paper 5178. https://doi.org/10.15760/etd.7054
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