Mechanistic biogeochemical model applications in the Florida Everglades

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Mechanistic vs. empirical modeling approaches

- Mechanistic models are based on the underlying physics and chemistry governing the processes and seek to describe phenomena with *transferable* equations that can be used predictively.
- This approach is contrasted with empirical methods that are based on observed relationships between variables that *may not be transferable* in space or time.
- The first step in developing a mechanistic model is to construct a conceptual model that defines the key interactions between process variables based on *fundamental* knowledge.
- Each interaction is then defined mathematically (e.g., first order, Monod, etc).
- Parameters for these relationships must then be obtained from experimental data.
- Finally the model should be validated against process data.
Model development in four easy steps…

• 1) Conceptual model, 2) Mathematical model, 3) Parameters, 4) Validate [4.5) Predict]
• Same steps whether empirical or mechanistic, differences appear in resilience to perturbations.
  – If model parameter (e.g., settling coefficient) is a function of load or vegetation community, then when these change, parameter must change
• What level of complexity is warranted? Perhaps consider model utility (management). Common to see model fits to data, but what predictions are desired? What hypotheses can be tested?
  – What if the external load is directly reduced? (e.g., Hg or TP) What about the effects of other controlling parameters? (e.g., SO4)
• But is it always mechanistic processes vs empirical?
  – Most models in use are hybrids where some processes are mechanistically/empirically described
Why pursue more complex models?

• Advantages of mechanistic approaches
  – not much data are required for model development
  – the model development process engenders “deep” knowledge of the system, and
  – the model parameters have physical meanings

• Disadvantages
  – development can be very time consuming and costly (but fundamentals are fundamentals)
  – solving the equations requires more sophisticated numerical techniques than simpler empirical approaches (perhaps big problems are worth a bit more effort)
  – adding new functionality requires fundamental understanding of the underlying processes (but new functionality _can be_ added)
A well known Everglades empirical model

Chemical engineering approach to phosphorus cycling in treatment wetlands: first order settling (e.g., Kadlec & Knight)

1) Conceptual Model

2) Mathematical Model

\[ \ln \left( \frac{C_1}{C_2} \right) = \frac{k_1}{q} \]

\[ \ln \left[ \frac{(C_1 - C^*)}{(C_2 - C^*)} \right] = \frac{k}{q} \]

- \(C_1, C_2\) = inlet/outlet concentrations
- \(C^*\) = background concentration
- \(k\) = settling rate
- \(q\) = hydraulic loading rate
Mechanistic model examples

Hg and P
Everglades Mercury Cycling Model (E-MCM)

- Dynamic process model to predict changes in mercury cycling and its biomagnification through aquatic food webs based on constructing a mercury mass balance. It simulates three different mercury forms and their interactions.
- The model includes a single compartment in the vertical for the water column and multiple sediment layers. The model can be applied as either single cell (i.e., unit wetland) or as a series of multiple linked cells.

MCM
(Developed for temperate lakes)

1997 - Ambrose et al. Screening Model
1998-99 E-MCM developed
Nov 1999 E-MCM workshop and model calibration to WCA 3A 15
April 2000 – Pilot Hg TMDL Completed
2000-2002: Calibration to additional sites and model improvements (FDEP, SFWMD)
2006-2007: Incorporation of Rodendiagenetic sub-model for sulfur dynamics in sediments
Overview of Hg Cycling in E-MCM
Bacterial Methylation [(SRB Activity = sulfate reducing bacteria activity)]

a.) Oxygenated Water Column  
b.) Anoxia in Water Column  
c.) Dry Conditions (no surface water)

Methylation Associated with Periphyton

a.) No Methylation  
b.) Methylation in anoxic zones  
c.) No Methylation

Figure 6. Conceptual model for methylation zones
Periphyton

Litter picks up atmospheric Hg (dry dep, RGM) and takes it to water column

Throughfall washes off during precip events

Roots pick up Hg(II), MeHg, Hg0 from porewater

Some reduction occurs as Hg(II) enters/passes through plants

Plants treated like single compartment with some extra Hg on leaves

Hg(II) reduced in via plant is transpired

Macrophyte Hg fluxes
Primary study sites where E-MCM has been applied
Predicted and observed total mercury concentrations (ng/L) in ENR surface waters: 4 years (unfiltered)
E-MCM calibration for Hg Tissue Concentrations in Largemouth Bass at Site 3A-15.

Figure 1. Total Hg emissions estimated for south Florida (Dade, Broward, and Palm Beach counties) for 1980 through 2000. Emissions based on plant operating data and emission factors. Source categories include municipal waste combustion (MWC), power generation, medical waste incineration (MWI), and sugar processing. From KMB Associates (2002).
Mechanistic Hg modeling considerations

- Surface sediments required to be very thin (3mm) to match observations
  - thin sediment = minimal buffering and leads to rapid water-column response to loading
  - quasi-empirical as perhaps other processes need refining
- Both Hg and SO4 loads were reduced. Model scenarios where either Hg or SO4 load was constant (not reduced) were evaluated
  - Hg reduction was found to be secondary to SO4 reduction in leading to reduced fish biomass Hg
  - But SO4 model is somewhat uncertain so hard to determine relative effects with confidence at this time
Mechanistic model examples

Hg and P
• Session 1: Poster 65 (Rajendra Paudel)  
Spatially distributed flow and phosphorus dynamics in STA1W

• Session 2, Posters 54/55 (Joong-Hyuk Min)  
Spatially distributed flow and phosphorus dynamics in STA 5/Ridge and slough
Appropriate level of complexity

- Simplest = one-parameter settling rate
- Complex = ecological succession models
- Intermediate = some physically-based processes, with lumping
- Coupled hydrologic and water quality modeling = many, many parameters
  “Make everything as simple as possible. But not simpler.”

*Albert Einstein*
Mesocosm Study (DB Environmental, 2006)

- Soil Depth, 20 cm
- Water Depth 40 cm
- Total Soil P
  - Cell 4 inflow region: 852 mg P kg$^{-1}$
  - Cell 4 outflow region: 273 mg P kg$^{-1}$
\[ G^{pl} = k_g^{pl} C^{pl} \frac{C^P_{sw}}{C^P_{sw} + k^{pl}_{1/2}} \]

Surface water SRP

\[ C^{TP}_{sw} \]

\[ \frac{dC^P_{sw}}{dt} = -k_{df} \frac{([C^P_{sw}] - [C^P_{pw}])}{z_{df}} \]

Porewater SRP

\[ C^P_{pw} \]

Plankton

\[ C^{pl} \]

\[ \frac{dC^{pl}}{dt} = k_{st}^{pl} [C^{pl}] \]

Soil

\[ S \]

\[ \frac{dS^o}{dt} = -k_{ox}^{so} S^o \]

\[ \frac{dS^p_{si}}{dt} = \rho_b f_i k^{sr}_d \frac{dC^P_{pw}}{\theta dt} \]
Mesocosm Study: Experimental and Model Results

- Level 1 processes: same parameters
  - $k_{ox} = 0.0015 \text{ day}^{-1}$
  - $k_{p\_growth} = 1 \text{ day}^{-1}$
  - $k_{p\_sn} = 0.28 \text{ day}^{-1}$
- Only difference between 2 cases is initial soil P
Managing South Florida treatment wetlands (STAs)

- STAs intercept agricultural runoff to reduce P load to Everglades
- What is the long-term sustainability of this $1B investment?
- Conceptual map of a management model
  - Tool for decision support
  - Scenario testing
  - Framework to integrate understanding and incorporate new understanding
STA1W Cell 4 simple ‘reactor model’– uptake and release

\[
\frac{dc(t)}{dt} = -k_u c(t) + \frac{k_r}{d} s(t)
\]

\[
\frac{ds(t)}{dt} = d k_u c(t) - k_r s(t)
\]
Figure 7. Comparison of cumulative phosphorus removal from SFWMD water sampling of inflow and outflow waters in Cell 4, to the phosphorus removal predicted by the model. SFWMD is South Florida Water Management District.

Figure 9. Measured and predicted change in soil P storage over time in the inflow and outflow region of Cell 4, as determined from soil phosphorus content and bulk density measurements of the newly accrued soil material (Irons, 2001). Values are mean ± 1 standard deviation of four soils per region.
STA1W-Cell 4: Hydrodynamic model

Field tracer test (Dierberg et al., 2005, Ecol. Eng.)

Tracer test simulation
STA1W-Cell4: Phosphorus model

\[
\frac{dC_{sw}^p}{dt} = -k_{sr}C_{sw}^p + k_{rs}S_p
\]

\[
\frac{dS_p}{dt} = k_{st}dC_{sw}^p + k_{rs}S_p
\]

Simulated soil P after 5 years
Animation of Total soil P distribution
Figure 14. Accumulated total soil phosphorus from samples collected at the end of 2000.
Total P concentration in WCA-2A soil (0-10 cm)
Total P concentration in WCA-2A soil (0-10 cm)

$T = 20\text{ yrs}$

$T = 30\text{ yrs}$
Soil and Water Science Department  
University of Florida  

Adsorbed Concentrations - 1. solute

T = 3, 15, 39, 66, 100, 133 years
Summary

• Mechanistic model development promotes better process understanding
• Process complexity should be represented appropriately
  – Flexible approaches recommended
• Capture hydrologic and biogeochemical complexity with spatially distributed models
• Hg deposition and SO4 loads reduced, fish concentration declined
  • uncertain: relative significance of SO4
• P accumulation in soils of treatment wetlands
  – What is long-term fate of P and treatment wetland lifespan?
    • uncertain: permanent burial/release of soil P