

Model Types

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What is a Water Quality Model?

A simplified, mathematical representation of pollutant fate and transport within a watershed and/or waterbody.





How to choose the right tool for the job

- Models can be thought of as tools to help you make informed decisions
- Your project has particular requirements
- Understanding the basic terminology, concepts and processes behind models is essential to choosing the right tool for the job







Empirical vs. Mechanistic Models

 Empirical (statistical) models rely upon the observed relationships among experimental data. They can be thought of as "best-fit" models



 Mechanistic (process) models explicitly include the mechanisms or processes between the state variables.



Empirical Models – Statistical Relationship





Empirical model - example

Universal Soil Loss Equation (USLE)

 $A = R \times K \times LS \times C \times P$

- Gets you from data observations to final estimate.
- Relatively simple to populate and understand.
- No real mechanistic value.
- No use of modeling concepts like mass balance.



Empirical Models – More Complex

- Multiple regression models
- Bayesian Analysis

$$P(A \mid B) = rac{P(B \mid A)P(A)}{P(B)}$$





Empirical Modeling - Summary

Pros

Cons

- Fast & easy
- Data requirements are likely small
- Links stressors to response variables

- Constrained by data availability/accuracy
- May not have confidence in the statistical fit
- Difficult to extrapolate to other situations
- May not account for all response variables



Mechanistic model - example

$$\Delta NO3_{str} = (\beta_{N,2} \cdot NO2_{str} - (1 - fr_{NH4}) \cdot \alpha_1 \cdot \mu_a \cdot algae) \cdot TT$$
7:3.2.10
Oxidation (increase) Uptake (decrease)

Clearly see the mechanisms underlying the model.

- Fundamentally based on conservation of mass, energy, and momentum.
- Many of the fundamental relationship were developed using direct observation.



Mechanistic Modeling - Summary

Pros

- Process linkage between stressors and response variables
- Extrapolate to other environmental conditions
- "Conservation" principles usually apply



Cons

Time consuming

Costly

Can be misapplied



Deterministic vs. Probabilistic Models

- Deterministic models provide a discrete solution. This type of model does not explicitly simulate the effects of data uncertainty or variability.
 Repeated simulations under constant conditions will result in consistent results.
- Probabilistic (or stochastic) models develop a probability distribution of model output rather than a single point value. Probabilistic models can be used to evaluate the impact of variability and uncertainty in the various input parameters.



Deterministic model - example

$$\Delta NO3_{str} = (\beta_{N,2} \cdot NO2_{str} - (1 - fr_{NH4}) \cdot \alpha_1 \cdot \mu_a \cdot algae) \cdot TT$$
7:3.2.10
Oxidation (increase) Uptake (decrease)

Same variables in the input = same result.



Stochastic model – example 1



- The model results show a probability distribution.
- Used when understanding risks may be more important than predicting a value.
- Actions can be based on desired level of confidence.



Stochastic model – example 2

- The model results multiple projected scenarios with variability for each scenario.
- Used when understanding risks may be more important than predicting a value.
- Actions can be based on desired level of confidence.





Static vs. Dynamic Models

- Static (steady state) models make predictions about the way a system changes as the value of an independent variable changes.
- Dynamic models make predictions about the way a system changes with time.
 Solutions are obtained by taking incremental finite time steps through the model domain.



Changes over time...

Steady-state model

- = snapshot in time
- = constant inputs and outputs



Mass Balance
 QUAL2K

Dynamic model

- = time varying
- = variable inputs and outputs





Simple vs. Complex Models

- Complex models...
- Require more data
- More computational power
- Cost more \$\$
- Are not always the best choice!

"Everything should be made as simple as possible, but no simpler." (Albert **Einstein**)



Simple vs. Complex Models



Photograph by Orren Jack Turner, Princeton, N.J.

"It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience." (Albert Einstein, 6/10/33)



Simple: Mass Balance on 1 Parameter



$$Q_{up} \cdot C_{up} + Q_{eff} \cdot C_{eff} = (Q_{up} + Q_{eff}) \cdot C_{down}$$

- Mixing instantaneous
- Conservation of mass assumed
- Steady state flows do not vary with time
- These are simplifications are they appropriate and defensible?

Complex: Linked Watershed and 3D Estuary Model for Multiple Parameters

• Mixing?

Conservation of mass?

Steady state?





When should you consider a...

...simple model?

- Few sources
- Not worried about pollutant speciation
- Steady state conditions
- Simple hydrology

...complex model?

- Multiple sources
- Complex pollutant response interactions
- Stratified waterbodies
- Fluctuating sources



Watershed Models vs Waterbody Models









Watershed Models

- Incorporate rainfall and runoff of water and dissolved materials on and through the land surface
- Erosion of sediment and associated constituents from the land surface
 Simple channel routing methodology.





Types of Water Quality Models Lumped vs. Semi-Distributed vs. Distributed

Refers to how the model considers spatial variability.



Source: Sitterson et. al, EPA/600/R-14/152, September 2017



Waterbody Models

- Rivers
- Lakes
- Estuaries
- Ocean/Coastal







Spatial Dimensions





Spatial Dimensions

- When is a 1-dimensional water quality model appropriate?
 - Free-flowing, well-mixed river or stream
- When is a 2-dimensional water quality model appropriate?
 - Shallow, well-mixed lake or estuary, or deep lake with little horizontal variability
- When is a 3-dimensional water quality model appropriate?
 - Deep reservoir or lake, wide poorly-mixed estuary







Public Domain Models (vs. Proprietary)

- Free
- Code/Manuals/Publications are available
- Peer Reviewed
- Limited tech support (you and internet searches)



Model Types - Summary

- Empirical vs. Mechanistic
- Deterministic vs. Probabilistic
- Static vs. Dynamic
- Simple vs. Complex
- Watershed vs. Waterbody



• Use your knowledge of model types to select the right model for your project!



Questions?

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