Broad Overview of Uncertainty Sources and Methods in Environmental Models

Kenneth Reckhow
Duke University

Is Scientific Knowledge Sufficient for Environmental Decision Making?

Yes, there is almost always enough scientific knowledge to make an informed decision.

And… these decisions may be expected to improve with information on the amount of scientific uncertainty and on public attitudes toward risk.

So, how do/should we make decisions when knowledge is uncertain?

How can knowledge of scientific uncertainty improve decision making?

Two essential elements that inform decision making:

- Probability model – this characterizes (scientific) knowledge; for example, this represents the prediction from a water quality model. Since it is probabilistic, it must include uncertainty analysis.

- Utility function – this characterizes the values of the decision makers (or stakeholders).

In theory, the *optimal* decision is found by integrating the probability model with the utility function.

This integration weights the utility (value) function by the probability of various outcomes.

This allows a risk-averse decision maker (through the utility function) to hedge against large losses.

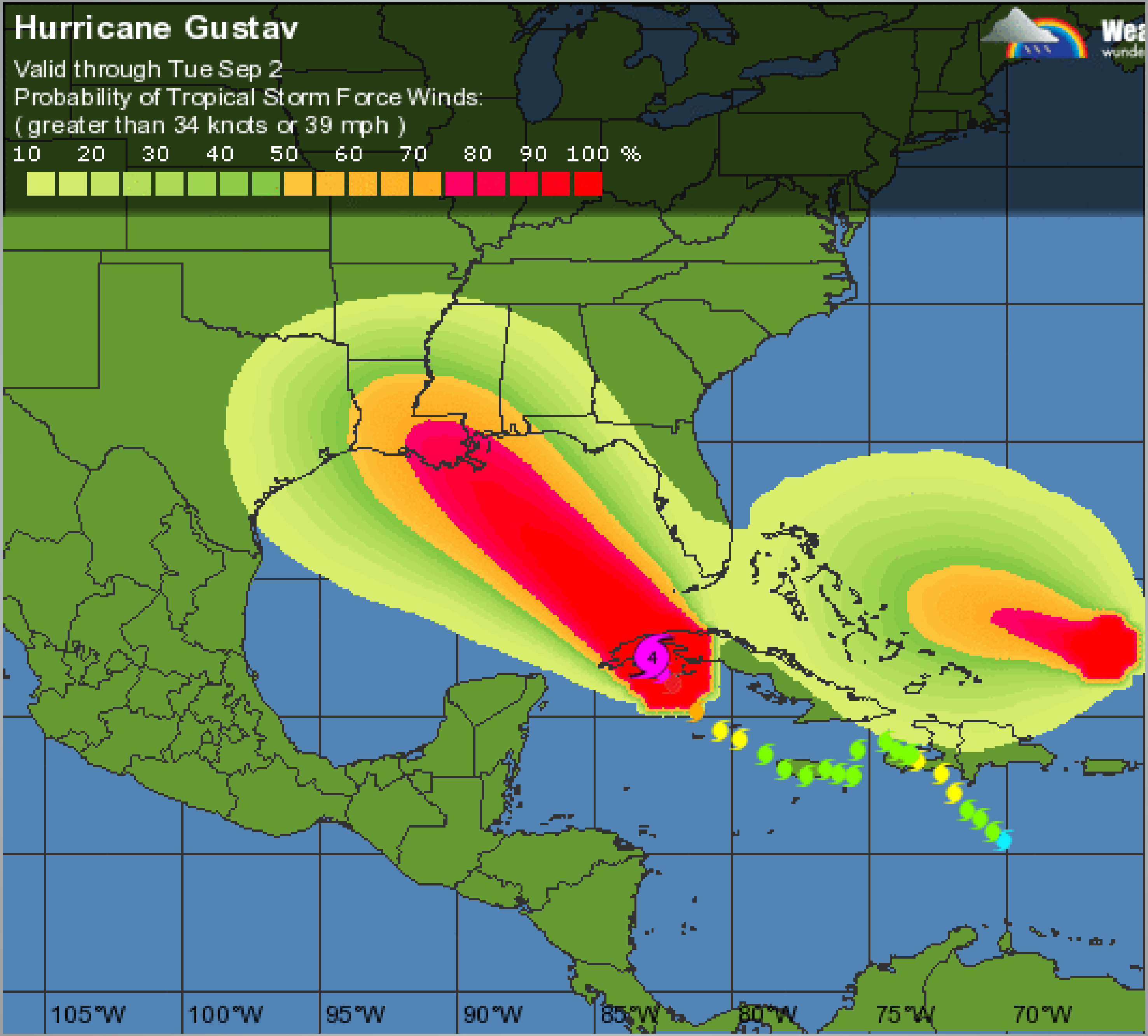
Only when the uncertainty in the scientific assessment (e.g., a WQ model) is determined, can the decision maker explicitly consider attitude toward risk.

8 DAY OUTLOOK

TUE	WED	THU	FRI	SAT	SUN	MON	TUE
49	46	58	73	75	73	70	70
80%	70%					40%	50%

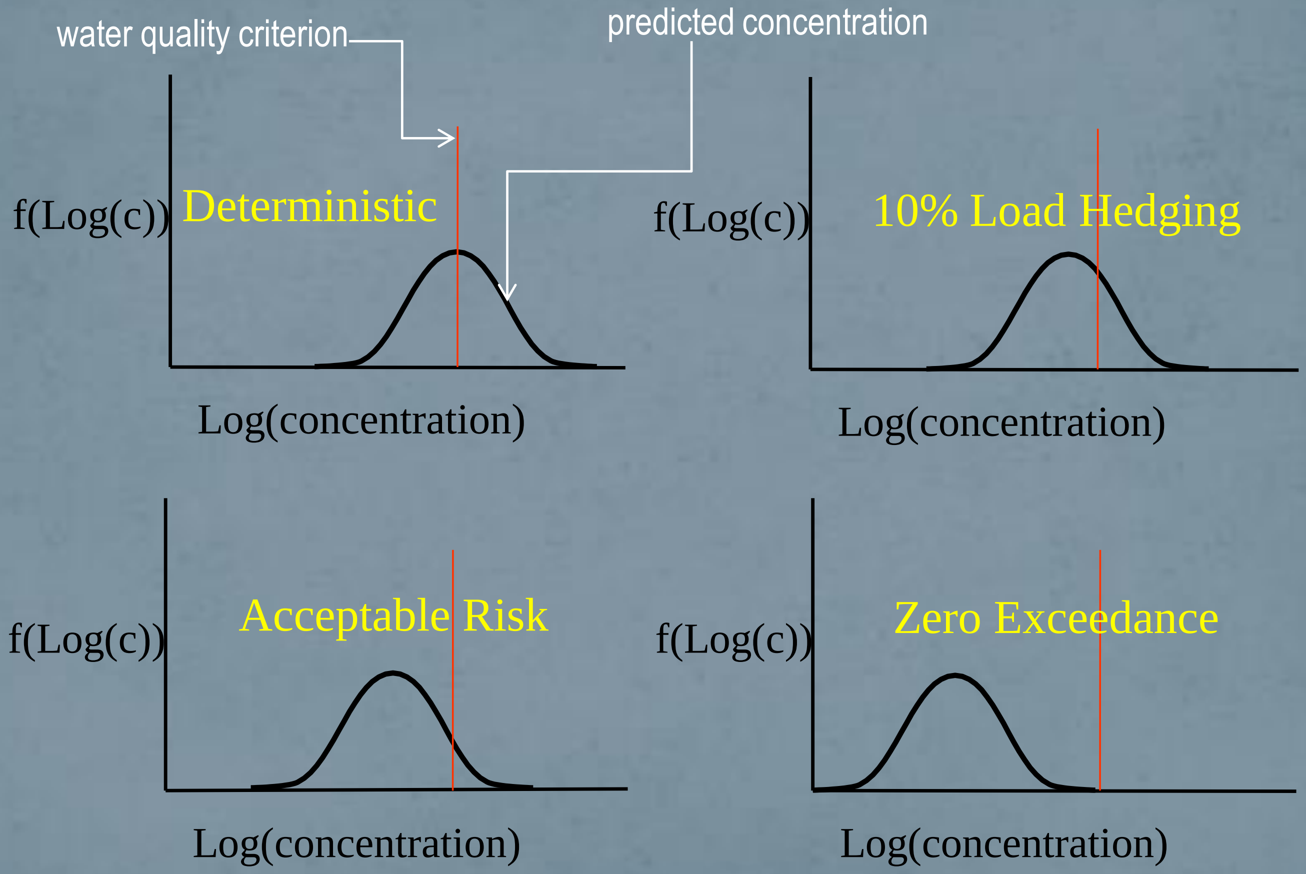
35 34 48 53 55 53 55

Much Warmer

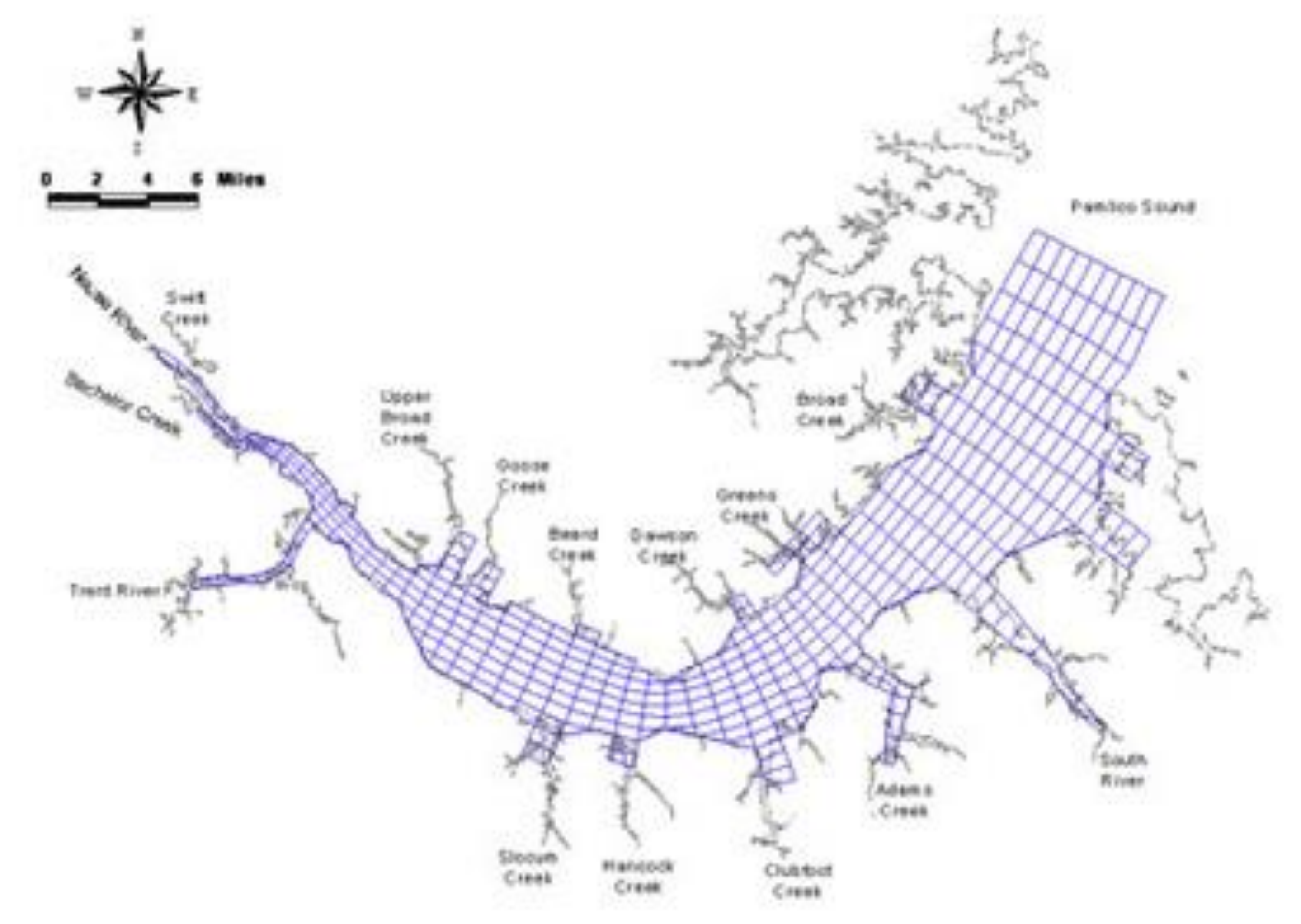

Hurricane Gustav
Valid through Tue Sep 2
Probability of Tropical Storm Force Winds:
(greater than 34 knots or 39 mph)
10 20 30 40 50 60 70 80 90 100 %
4
105°W
100°W
95°W
90°W
85°W
80°W
75°W
70°W

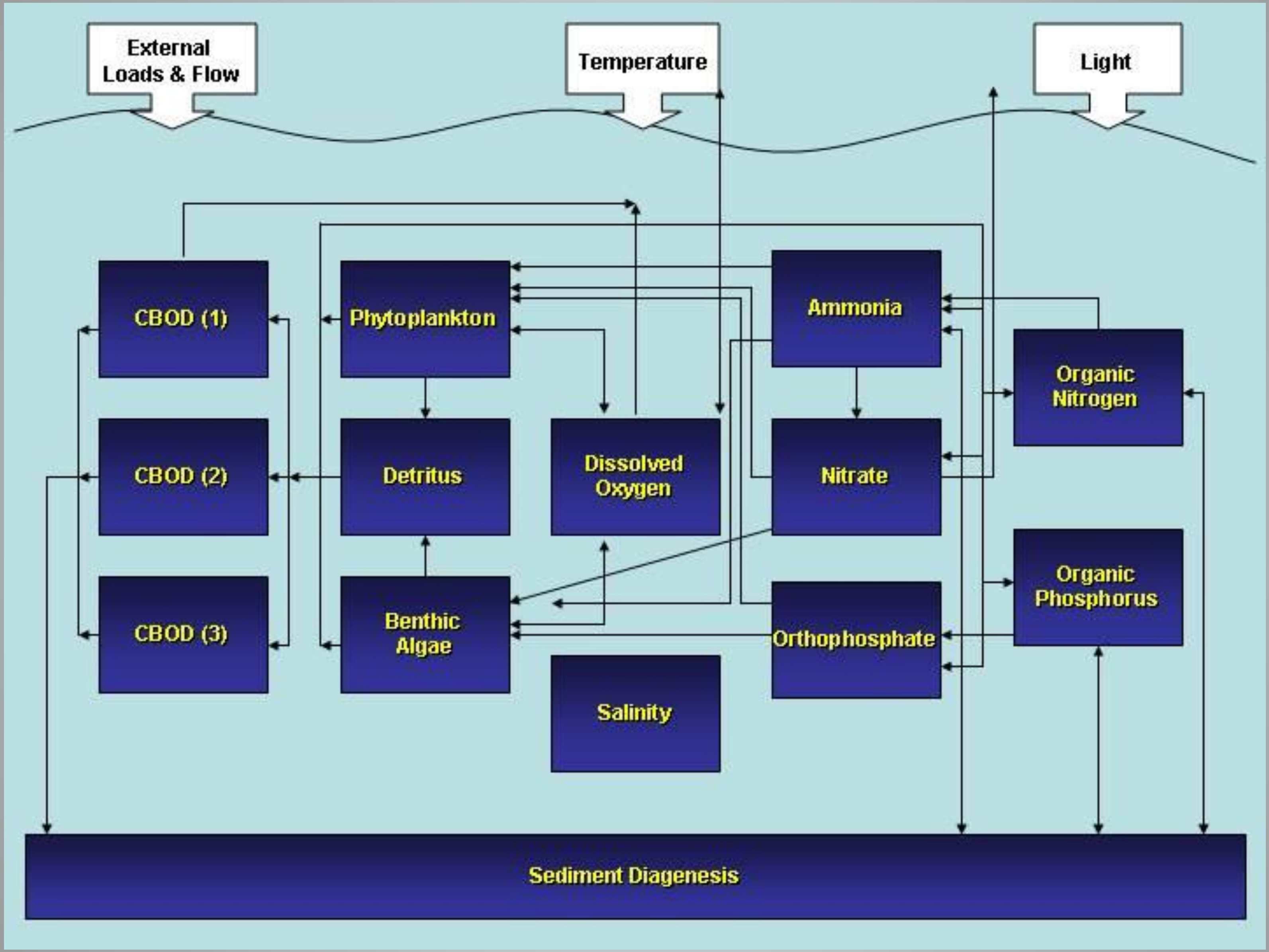
How do you want it – the crystal mumbo-jumbo
or statistical probability?

EPA TMDL Approval: Four Scenarios



An illustration of my concerns about highly-detailed mechanistic models





External Loads & Flow

Temperature

Light

CBOD (1)

Phytoplankton

Ammonia

Organic Nitrogen

CBOD (2)

Detritus

Dissolved Oxygen

Nitrate

Organic Phosphorus

CBOD (3)

Benthic Algae

Orthophosphate

Salinity

Sediment Diagenesis

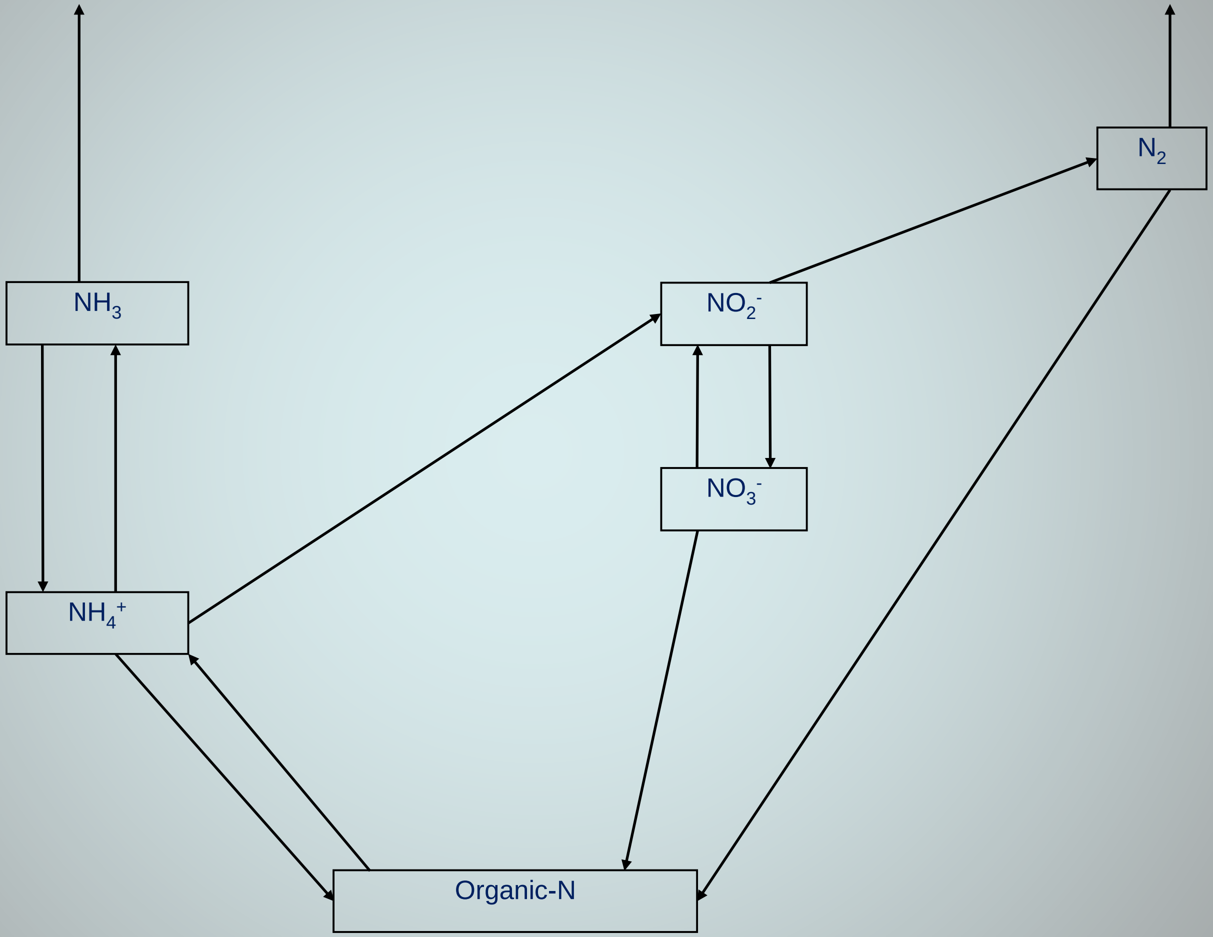
Some Important Issues

- How do we know that mechanistic WQ models represent reality?

- Is “getting the processes right” an achievable goal?

- What can we learn from decision analysis about the nature of scientific analysis to guide decision making under uncertainty?

Consider modeling of chemical reactions



NH_3

NO_2^-

N_2

NO_3^-

NH_4^+

Organic-N

Parameter Estimation/Selection in WQ Models

- Mechanistic (process) models
  - *measure* - physically-based models

  - *choose* - using the User’s Manual or “Rates” Manual

- Statistical (empirical) models
  - *optimize* - least squares, maximum likelihood

- Recent developments (equifinality)
  - *simulate* - estimate parameter distributions (RSA, GLUE, MCMC)

Mechanistic Model Equation: Phytoplankton Settling Velocity

$$\frac{dVC_1}{dt} = QC_{in} + EA\frac{dC_1}{dt} - QC_1 + (\mu_1 - R_1 - M_1)VC_1 - \mu_2 VC_2 F_{2,1} - v_1 AC_1$$

Where:

V = segment volume (m^3)
C_1 = phytoplankton concentration (g/m^3)
Q = flow volume (m^3/t)
E = diffusion coefficient (m^2/t)
A = segment surface/bottom area (m^2)
μ_1 = phytoplankton growth rate (t^{-1})
R_1 = phytoplankton respiration rate (t^{-1})
v_1 = phytoplankton settling velocity (m/t)
M_1 = phytoplankton mortality rate (t^{-1})
μ_2 = zooplankton growth rate (t^{-1})
C_2 = zooplankton concentration (g/m^3)
$F_{2,1}$ = fractional feeding preference

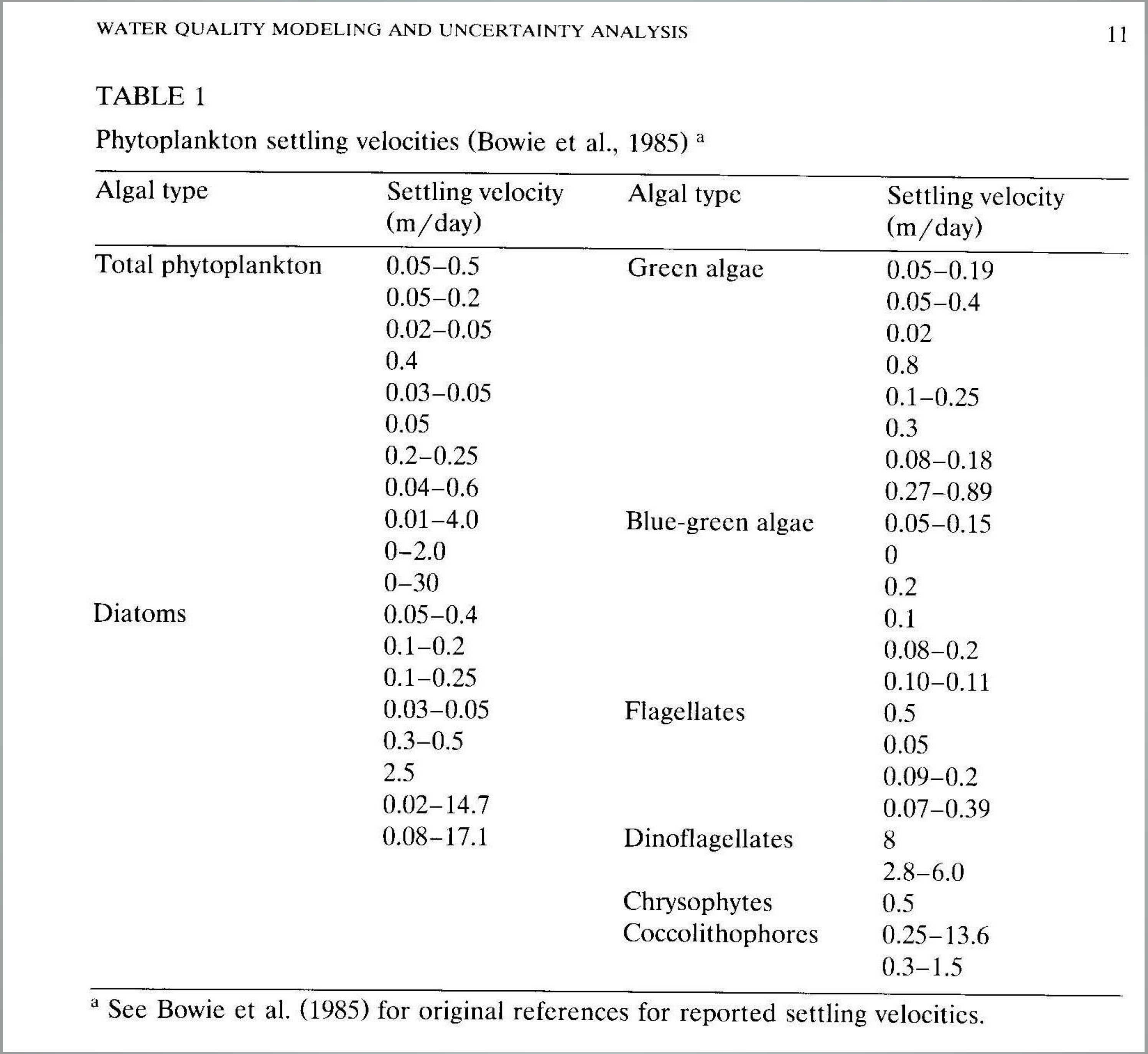


TABLE 1

Phytoplankton settling velocities (Bowie et al., 1985) [a]

Algal type	Settling velocity (m/day)	Algal type	Settling velocity (m/day)
Total phytoplankton	0.05–0.5	Green algae	0.05–0.19
	0.05–0.2		0.05–0.4
	0.02–0.05		0.02
	0.4		0.8
	0.03–0.05		0.1–0.25
	0.05		0.3
	0.2–0.25		0.08–0.18
	0.04–0.6		0.27–0.89
	0.01–4.0	Blue-green algae	0.05–0.15
	0–2.0		0
	0–30		0.2
Diatoms	0.05–0.4		0.1
	0.1–0.2		0.08–0.2
	0.1–0.25		0.10–0.11
	0.03–0.05	Flagellates	0.5
	0.3–0.5		0.05
	2.5		0.09–0.2
	0.02–14.7		0.07–0.39
	0.08–17.1	Dinoflagellates	8
			2.8–6.0
		Chrysophytes	0.5
		Coccolithophores	0.25–13.6
			0.3–1.5

[a] See Bowie et al. (1985) for original references for reported settling velocities.

Uncertainty Analysis in WQ Models

- First-order error analysis
- Monte Carlo simulation
- Recent developments (addressing equifinality) that focus on parameter distribution estimation

First Order Error Analysis

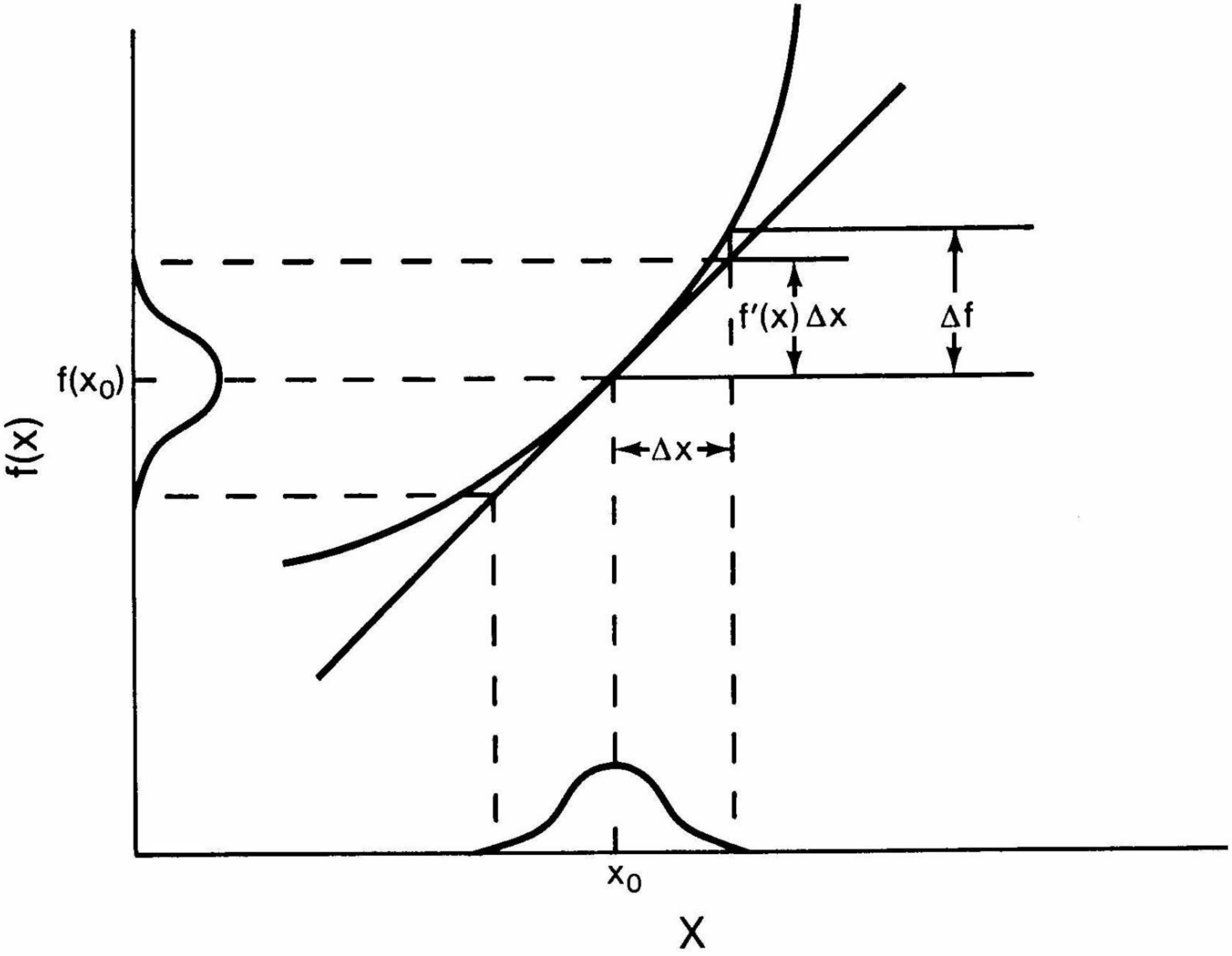
Model: $y = b_0 + b_1x$

Error propagation equation:

$$s_y = \frac{\partial y}{\partial x} s_x$$

For a multivariate equation:

$$s_y^2 \sim \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i}\right)^2 s_{x_i}^2 + 2 \sum_{j=1}^{n-1} \sum_{i=j+1}^{n} \left(\frac{\partial f}{\partial x_i}\right)\left(\frac{\partial f}{\partial x_j}\right) s_{x_i} s_{x_j} \rho_{x_i x_j}$$

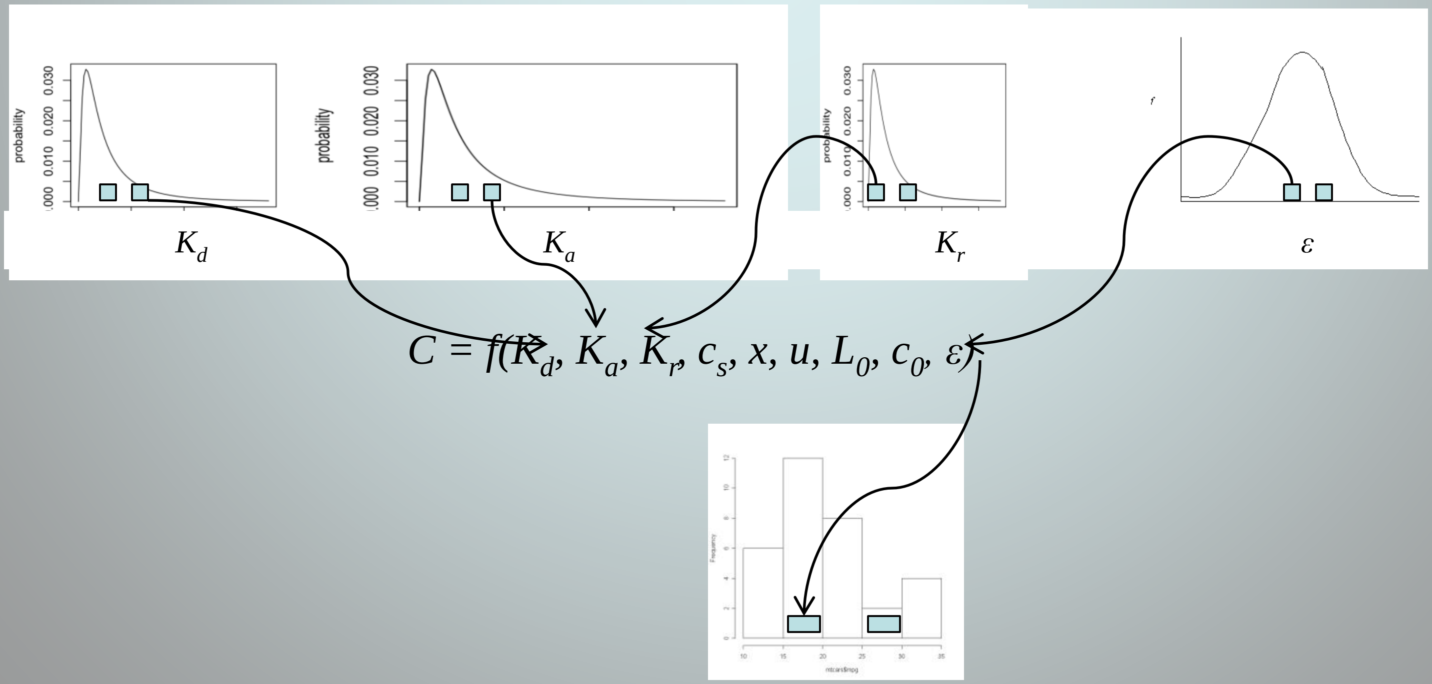

f′(x) Δx
Δf
f(x₀)
f(x)
Δx
x₀
X

Monte Carlo Simulation

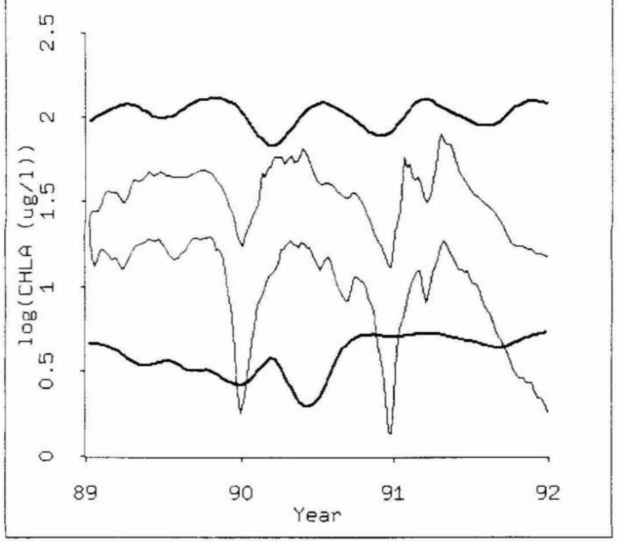
Dissolved Oxygen Stream Model

$$C = C_s - \left[\frac{K_d}{K_a - K_r}\left(e^{\frac{-K_r x}{u}}\right) - \left(e^{\frac{-K_a x}{u}}\right)\right] L_0 - (c_s - c_0)e^{\frac{-K_a x}{u}} + \varepsilon$$

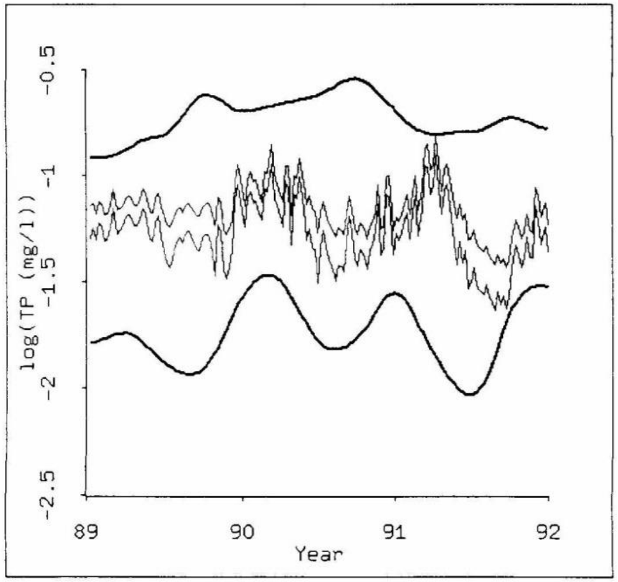
Assume that uncertainty in the model is characterized by:



$C = f(K_d, K_a, K_r, c_s, x, u, L_0, c_0, \varepsilon)$



RSA Simulation to estimate parameter distributions



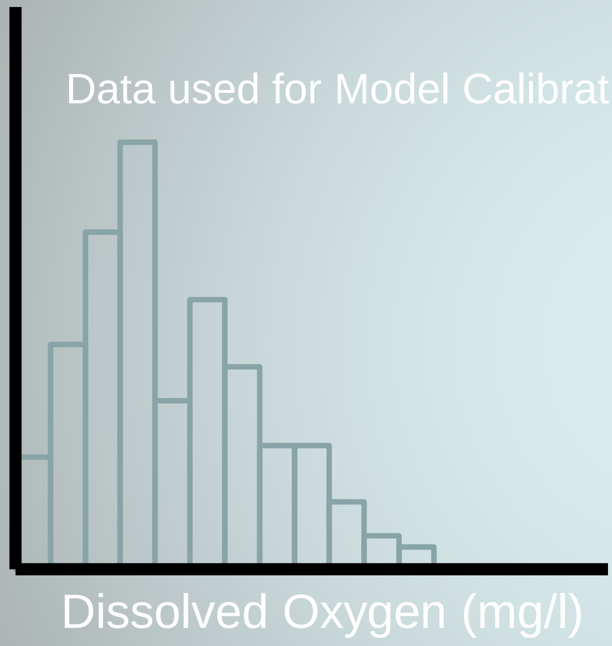
Skill Assessment:
The Direct Comparison of Model Predictions and Observations

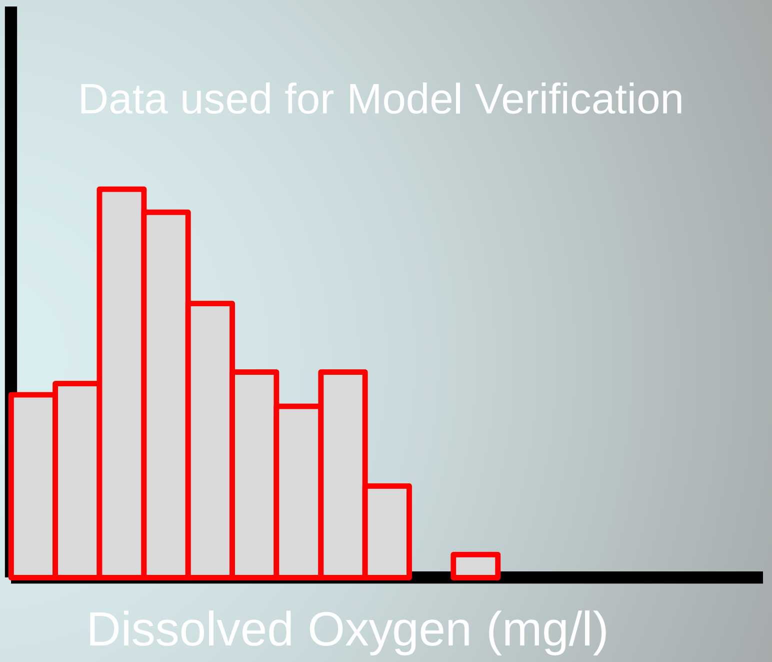
“Skill assessment” for water quality models refers to the results of a set of statistical and graphical techniques to quantify the goodness-of-fit for a water quality model. The t-test, the Wilcoxon test, regression analysis, and the Kolmogorov-Smirnov test are often recommended for the “verification” of a mechanistic water-quality model.

Reckhow, K.H., J.T. Clements, and R.C. Dodd. 1990. Statistical evaluation of mechanistic water quality models. *Journal of Environmental Engineering.* 116:250-268.

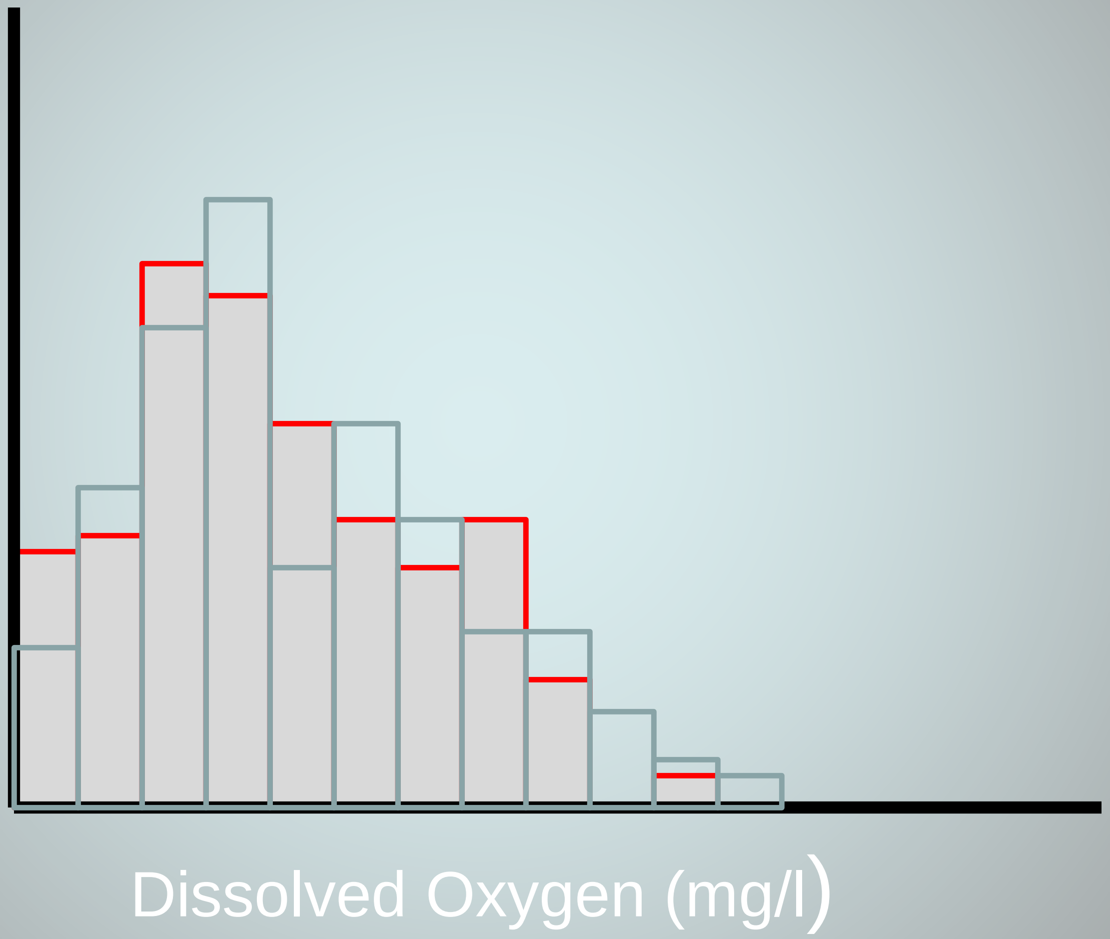
Stow, C.A., J. Jolliff, D.J. McGillicuddy, S.C. Doney, J.I. Allen, M.A.M. Friedrichs, K.A. Rose, and P. Wallhead. 2009. Skill assessment for coupled biological/physical models of marine systems. *Journal of Marine Systems* 76:4-15.

Evaluation of the Strength and Importance of Model Verification
Case 1

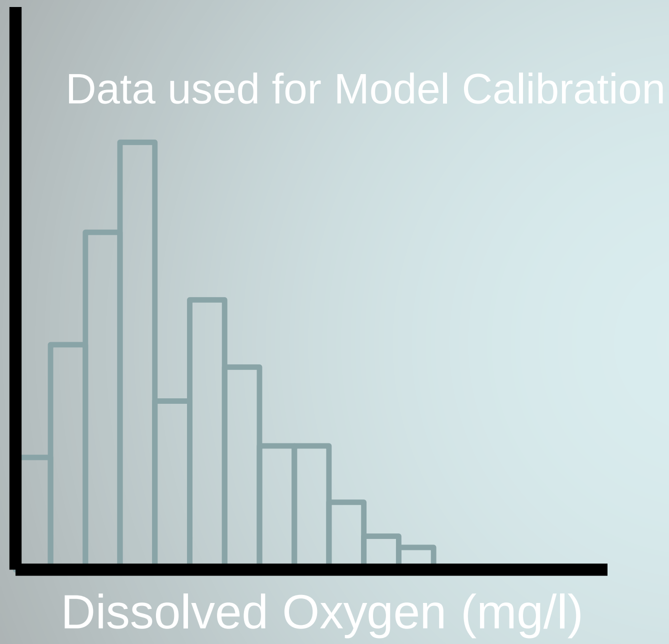


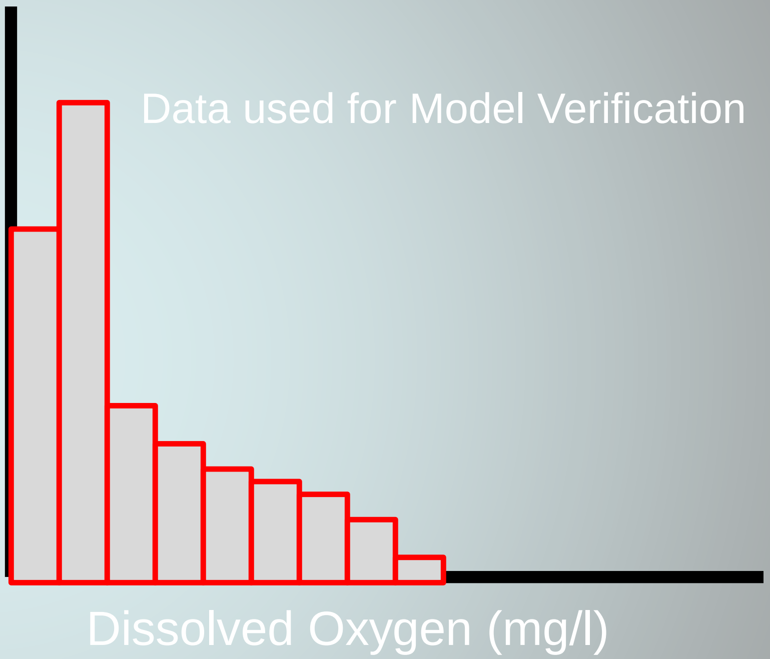


Calibration and Verification Data Comparison: Case 1

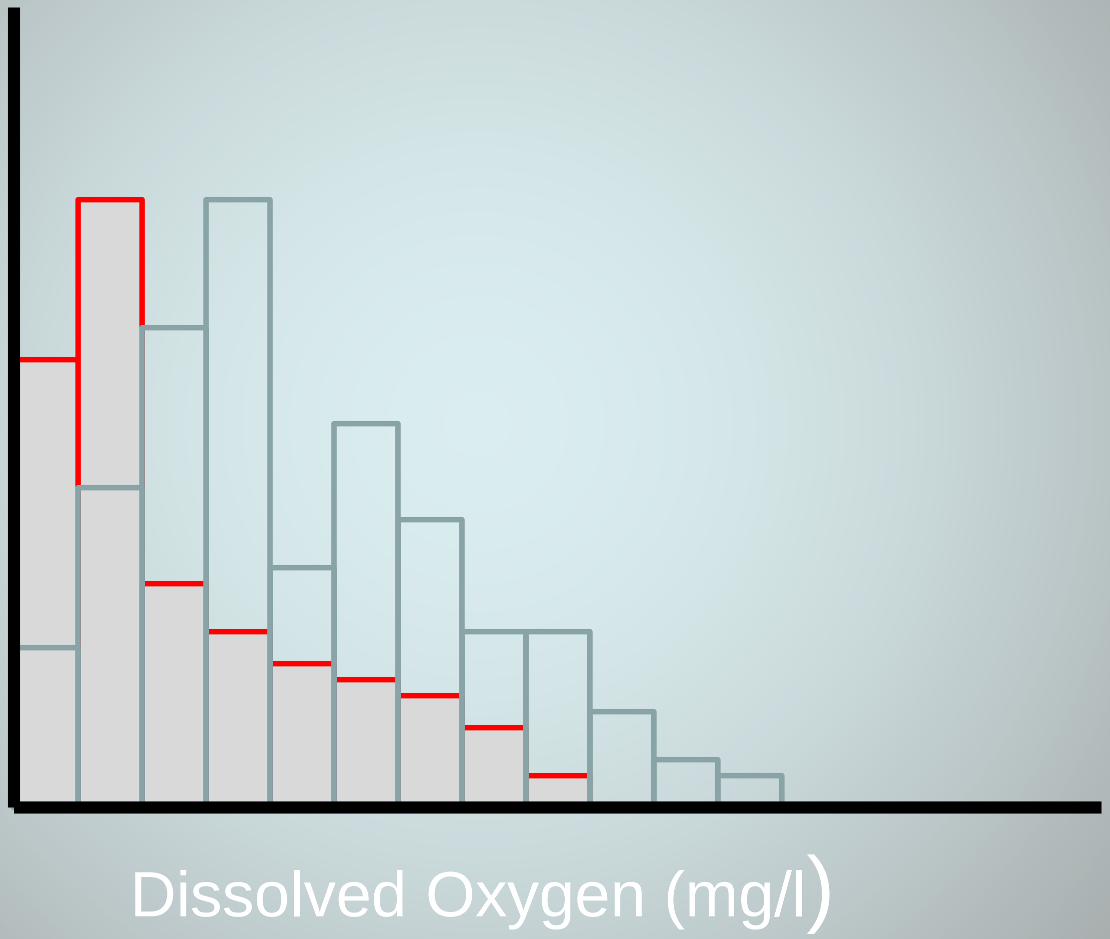


Evaluation of the Strength and Importance of Model Verification
Case 2

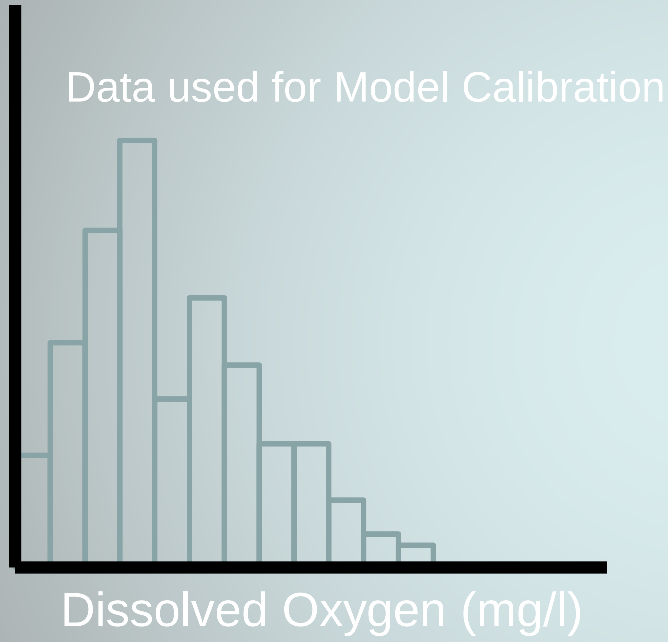


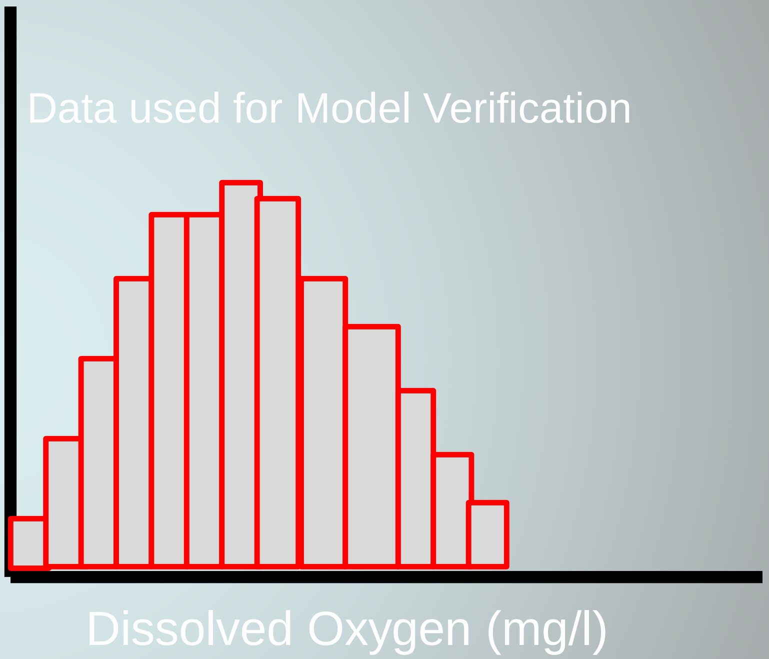


Calibration and Verification Data Comparison: Case 2

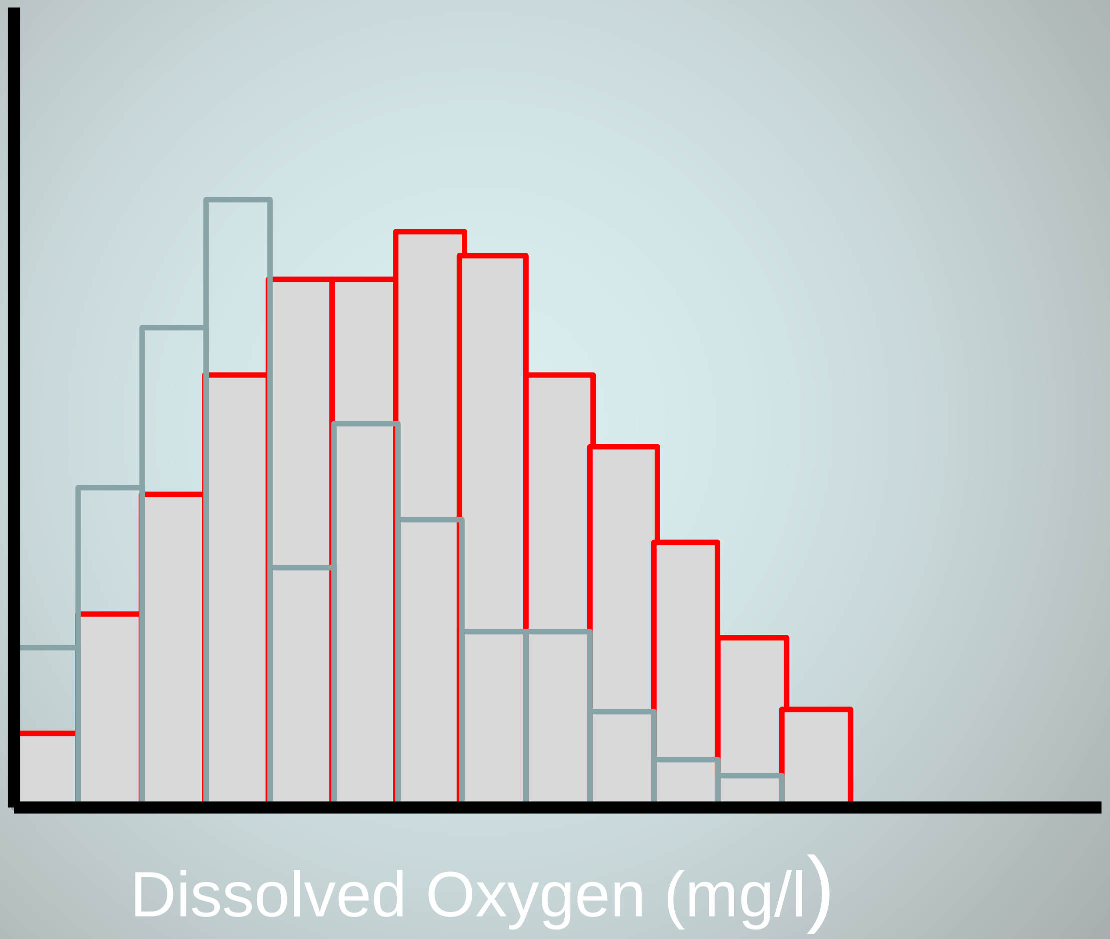


Evaluation of the Strength and Importance of Model Verification
Case 3





Calibration and Verification Data Comparison: Case 3



Research & Application Challenges

How can we quantify prediction uncertainty for complex models?

How can we present uncertain science to decision makers and stakeholders so that they make better decisions than they would in the absence of knowledge of uncertainty?

"There's a 50% chance of rain, so I only watered half the lawn."

Given the uncertainty, how do we decide?

We can “learn while doing;” that is, we can observe how the real system (the actual waterbody) responds, and then use that information to augment and improve the prediction for the modeled system.

Why does this approach make sense?

- If model forecasts are highly uncertain, then chances are high that adjustments will be necessary (i.e., we’ll likely get it wrong on the first try).

- If we know that we’re likely to be wrong with the initial assessments, then it makes sense to develop and implement the pollutant load reductions to help determine the future adjustments to the reductions.


NCAA
2015 DIVISION I
MEN'S BASKETBALL
NATIONAL CHAMPION
NATIONAL CHAMPIONS
2015 NCAA
MEN'S BASKETBALL
CHAMPIONS