Surface Water Quality Modeling

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https://triton.wasser.tum.de/

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Water quality under climate change

Water quality under climate change

Content

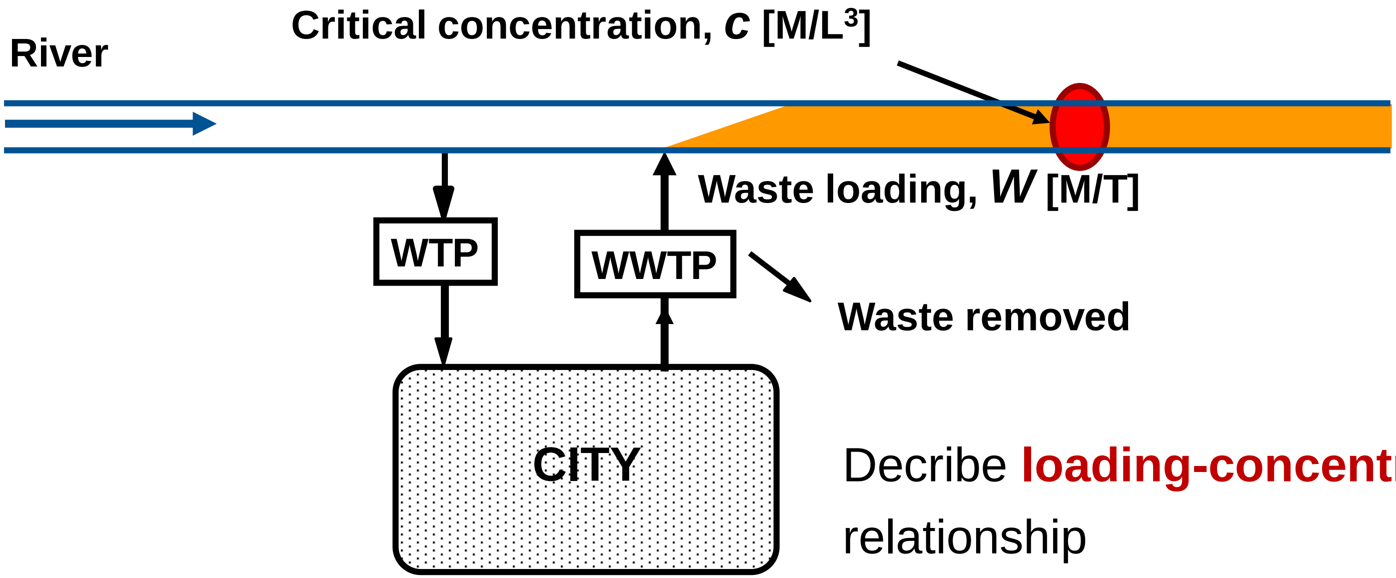
1. Introduction to Water Quality Modeling
   – What is water quality modeling?
   – Mass balance
   – Analytical & numerical solutions
2. Kinetics
   – Zero & first-order reactions
   – Temperature effects
3. Applications

FARADAY GIVING HIS CARD TO FATHER THAMES;
And we hope the Dirty Fellow will consult the learned Professor.

P1. Introduction to Water Quality Modeling

- ***What is water quality modeling?***
- ***Mass balance***
- ***Analytical & numerical solutions***

URBAN POINT SOURCE DESIGN PROBLEM (Circa 1920s)

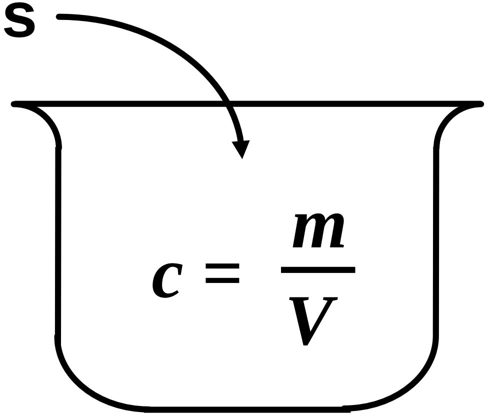


Decribe **loading-concentration** relationship

WATER-QUALITY MODEL: $c = f(W$, **physics, chemistry, biology)**

MASS AND CONCENTRATION

m = mass

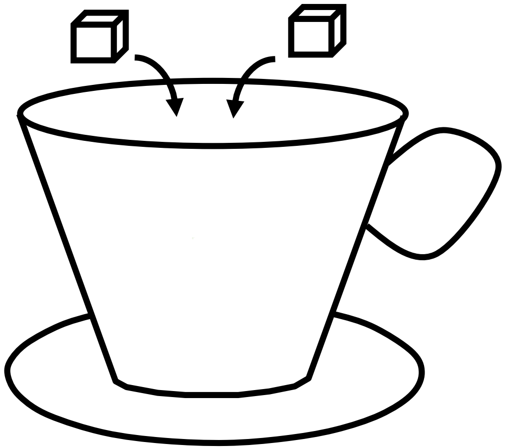


$$c = \frac{m}{V}$$

V = volume

units: $\frac{\mathrm{M}}{\mathrm{L}^3}$

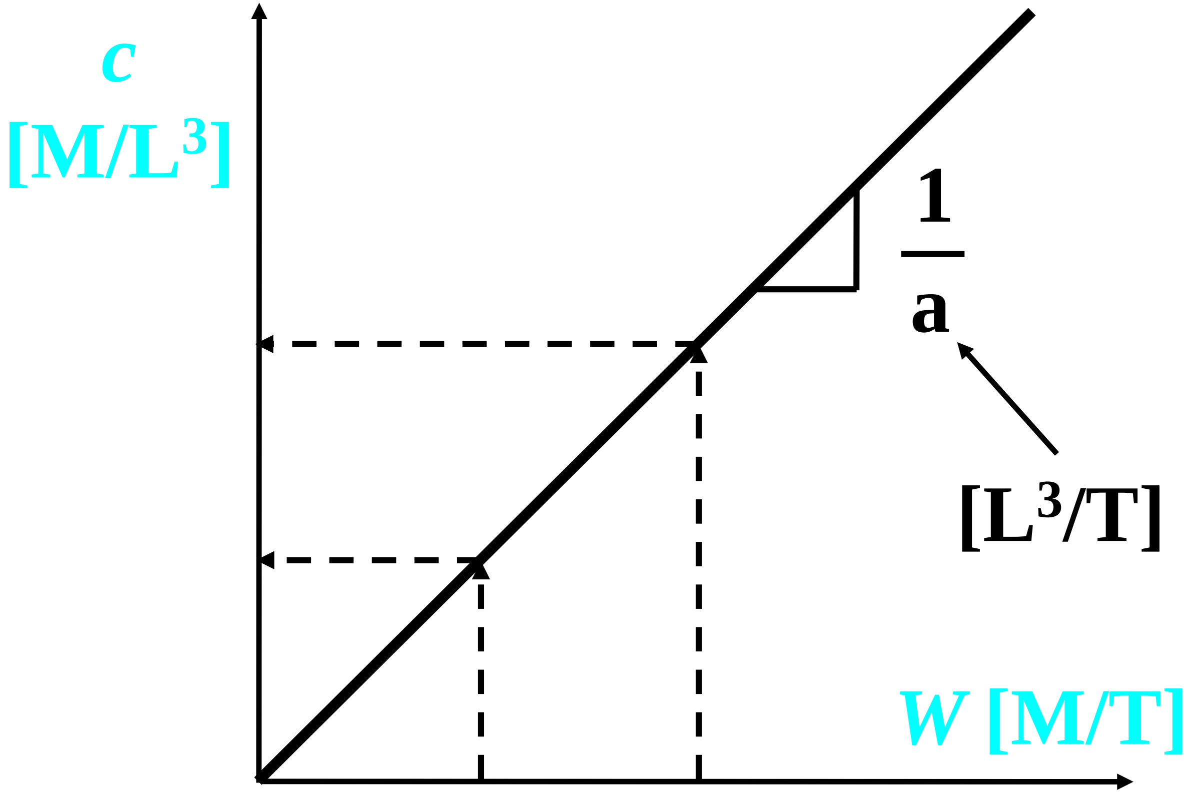
note: **M =** ***mass*****, L =** ***length*****, T =** ***time*****, H =** ***heat***



MASS → AMOUNT OF SUGAR

CONCENTRATION → SWEETNESS

SIMPLE LINEAR MODEL



ASSIMILATION FACTOR

$$c = \frac{1}{a}\,W$$

$$\xrightarrow{\;W\;} \boxed{\frac{1}{a}} \xrightarrow{\;c\;}$$

$$\textbf{stimulus} \rightarrow \underbrace{\textbf{system}}_{\text{physics, chemistry, biology}} \rightarrow \textbf{response}$$

MODELING MODES

SIMULATION MODE: Given load (W) and assimilation factor (a), calculate

$$c = \frac{1}{a} W$$

ASSIMILATIVE CAPACITY DESIGN MODE: Given desired concentration (c) and assimilation factor (a), calculate

$$W = a\,c$$

ENVIRONMENTAL MODIFICATION DESIGN MODE: Given desired concentration (c) and load (W), calculate

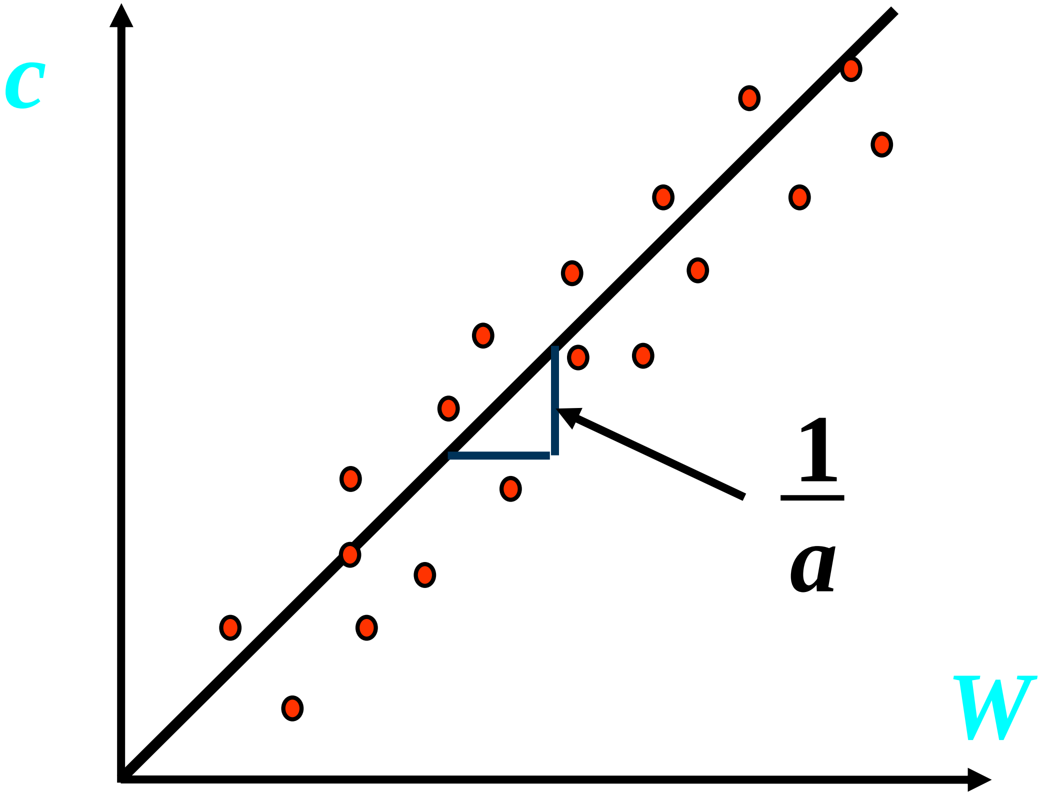
$$a = \frac{W}{c}$$

HOW DO WE DETERMINE “*a*”?

EMPIRICAL
Data-based
(Inductive,
Statistical)
Model

MECHANISTIC
Process-based
(Deductive
Mass-balance)
Model

EMPIRICAL MODELS



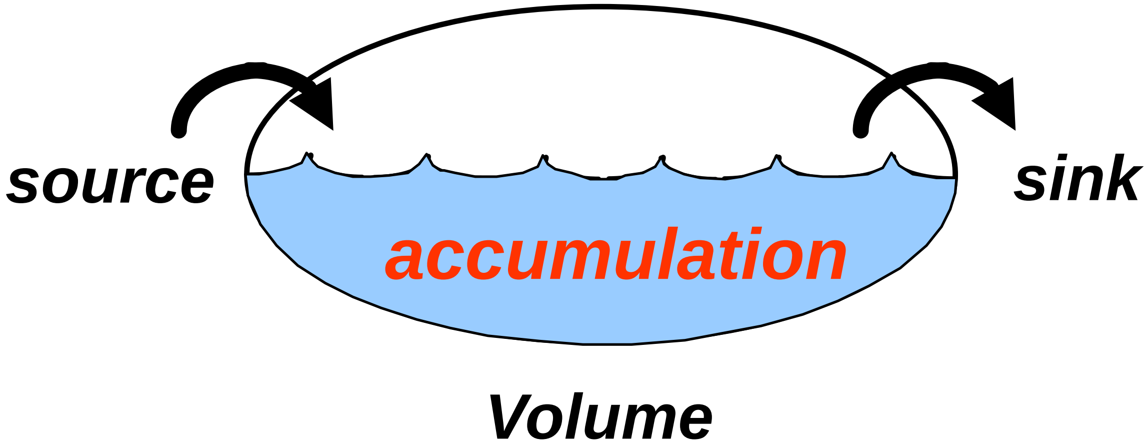
MECHANISTIC MODELS

CONSERVATION OF MASS

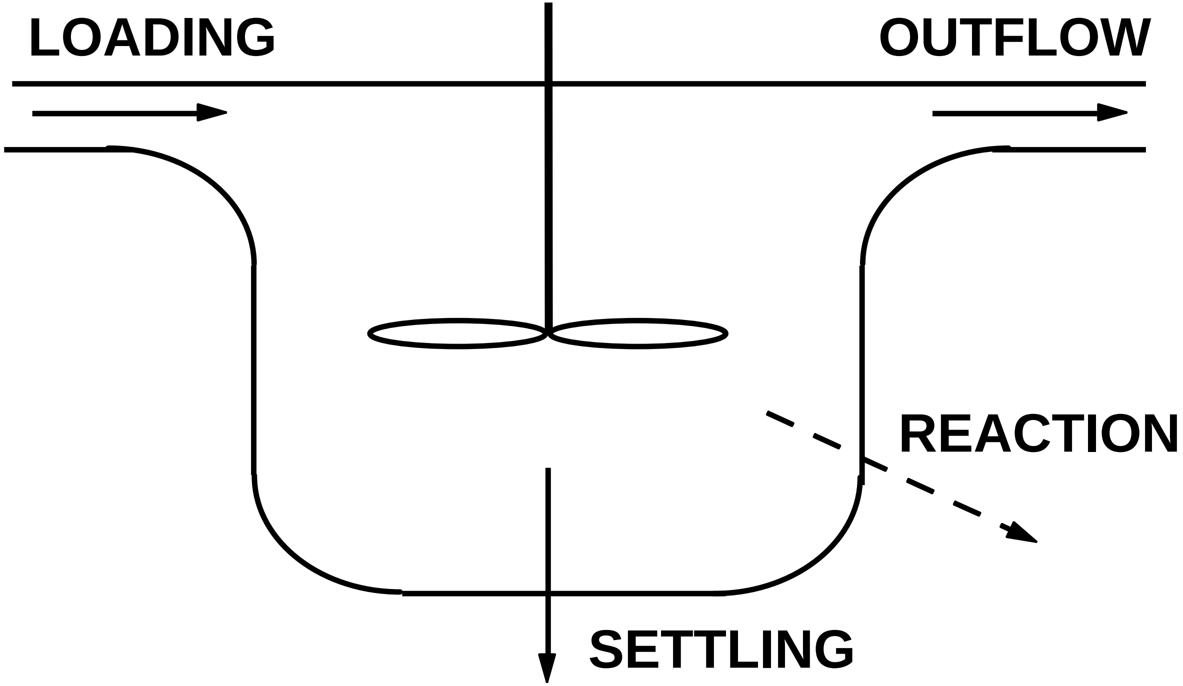
Mass Balance:

For a finite volume over a unit time period:

(accumulation) = (sources) – (sinks)



MASS BALANCE FOR WELL-MIXED LAKE



ACCUMULATION = LOADING − OUTFLOW − REACTION − SETTLING

PARAMETERIZE ACCUMULATION

$$\text{accumulation} = \frac{\Delta M}{\Delta t}$$

Substitute $M = Vc$

$$\text{accumulation} = \frac{\Delta Vc}{\Delta t}$$

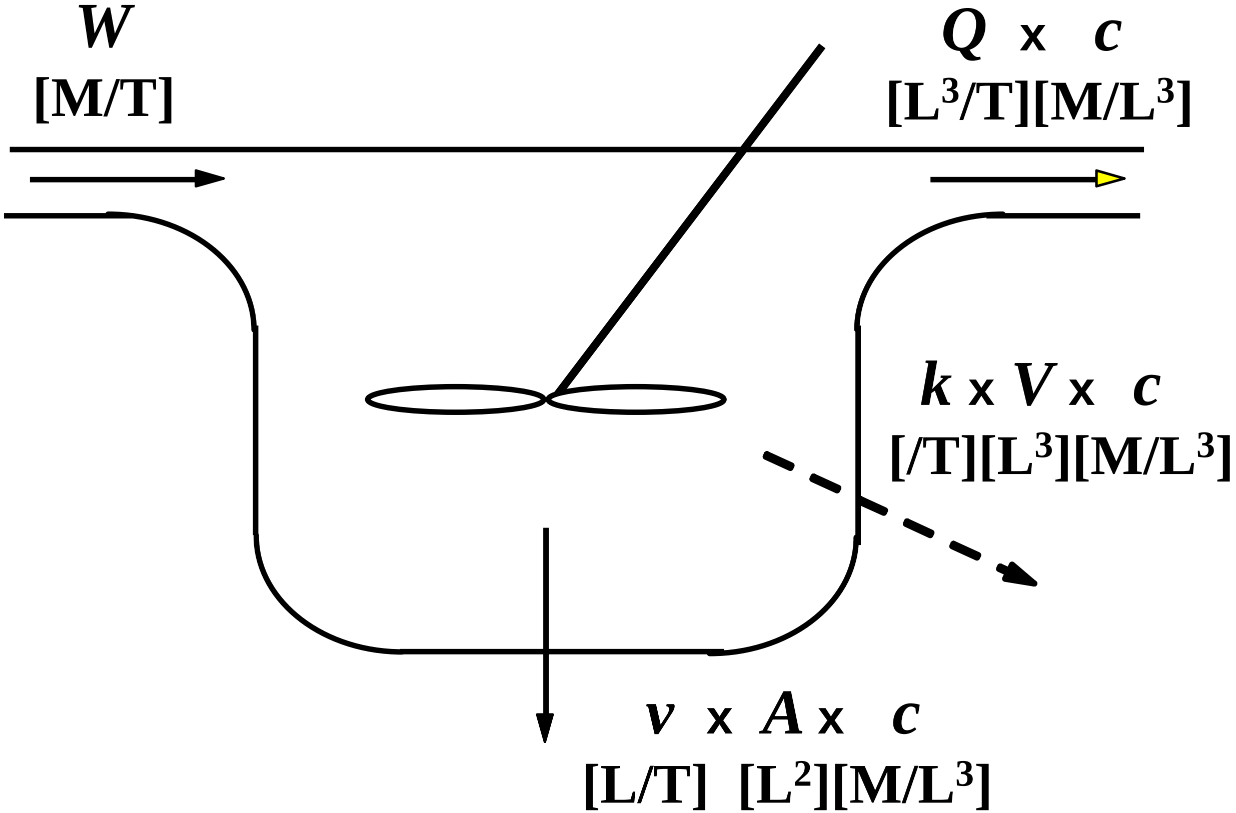
If V = constant

$$\text{accumulation} = V\frac{\Delta c}{\Delta t}$$

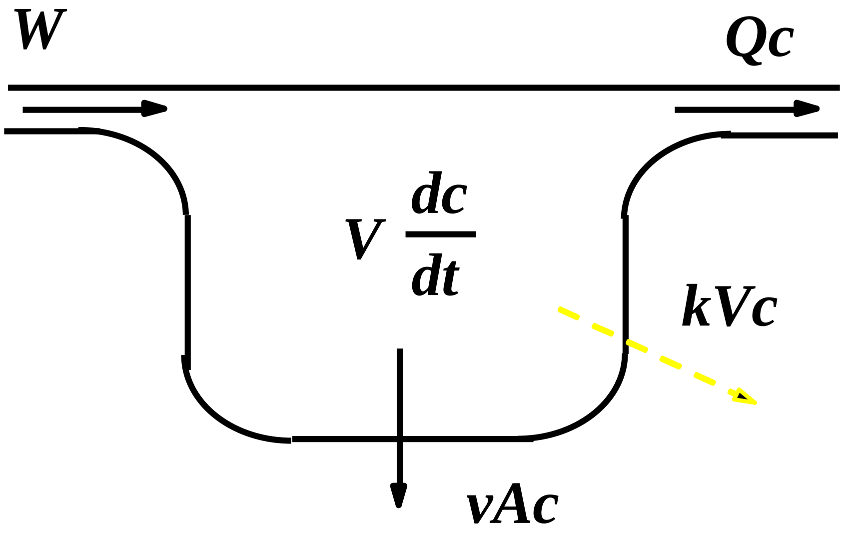
Let $\Delta t \longrightarrow 0$

$$\boxed{\text{accumulation} = V\frac{dc}{dt}}$$

PARAMETERIZE SOURCE/SINK MECHANISMS



MASS-BALANCE EQUATION



$$V\frac{dc}{dt} = W - Qc - kVc - vAc$$

accumulation = load – outflow – reaction – settling

THE FINAL MODEL

A single, linear, first-order, nonhomogeneous ordinary differential equation

$$V\frac{dc}{dt} = W - Qc - kVc - vAc$$

Canonical form:

dependent variable

$$\frac{dc}{dt} + \left(\frac{Q}{V} + k + \frac{v}{H}\right)c = \frac{W}{V}$$

independent variable

parameters

forcing function

SOLUTIONS

- ***Steady-state (Accumulation = 0)***

  What happens if we subject a system to constant conditions for a sufficiently long period? What will be the stable state?

- ***Time-variable or transient solutions***

  Given an initial condition, how will the system change temporally?

STEADY-STATE SOLUTION

$$V\cancel{\frac{dc}{dt}}^{0} = W - Qc - kVc - vAc$$

$$\boxed{c = \frac{W}{Q + kV + vA}}$$

Forcing function (The "external" world)

Purging parameters (physics, chemistry, biology)

WE'VE NOW DERIVED THE ASSIMILATION FACTOR!!!

$$c = \frac{W}{Q + kV + vA}$$

$$c = \frac{1}{a} W$$

a = assimilation factor

$= Q + kV + vA$

physics

chemistry, biology

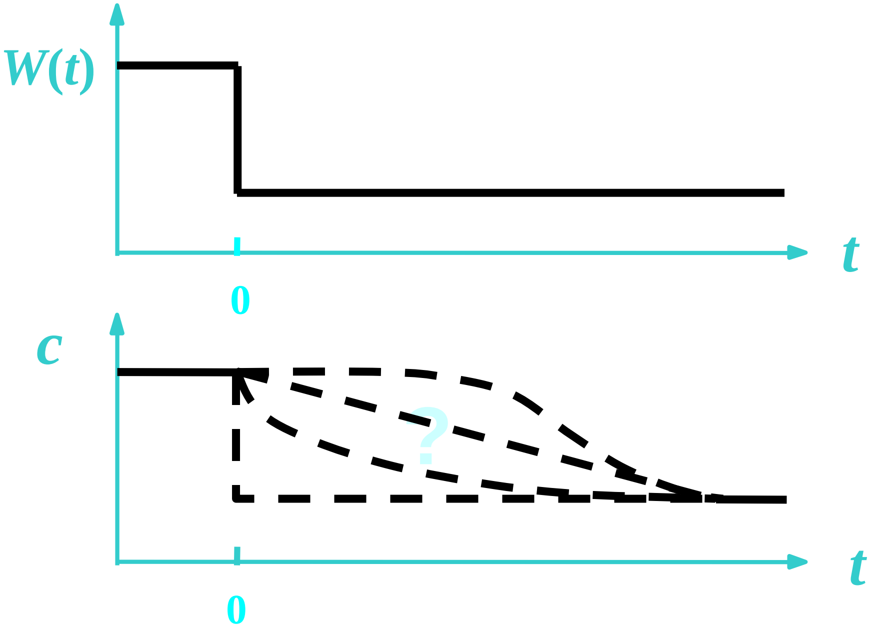
"transport"

"kinetics"

TEMPORAL ASPECTS OF POLLUTANT REDUCTION

Questions:

- ***How long will it take for improvement to occur?***
- ***What will the shape of the recovery look like?***



TIME-VARIABLE SOLUTIONS
ANALYTICAL VS. NUMERICAL

$$\frac{dc}{dt} + \lambda c = \frac{W(t)}{V}$$

analytical (closed form)	numerical
calculus	computer
continuous	discrete
equation	table of values

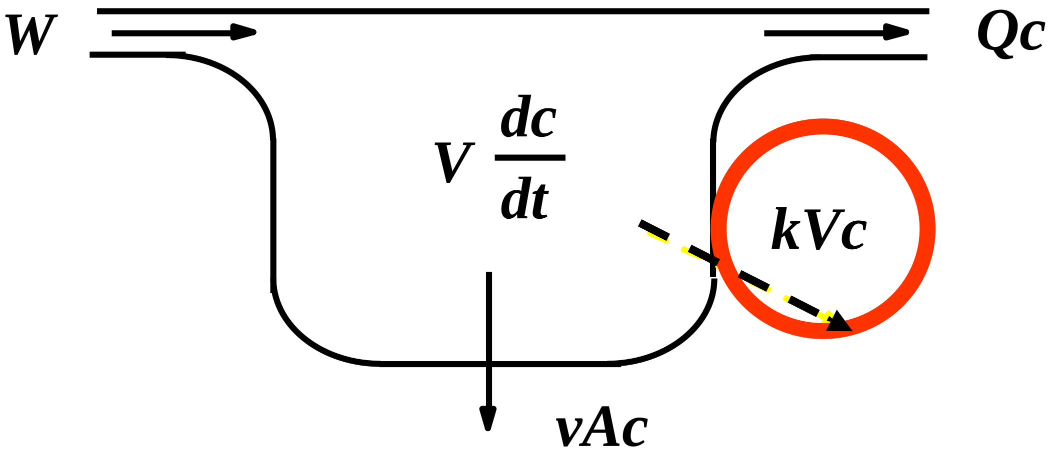
IF WE HAVE COMPUTERS:
WHY ANALYTICAL SOLUTIONS???

- Great for insights and fundamental understanding
  - For example, dimensionless numbers
- Quick assessments
  - “Back of the envelope” calculations
- Useful for checking numerical computer solutions

P2. REACTION KINETICS

- ***Kinetics***
  - ***Zero & first-order reactions***
  - ***Temperature effects***

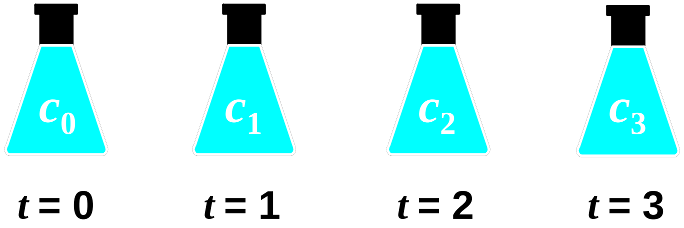
MASS-BALANCE FOR WELL-MIXED LAKE



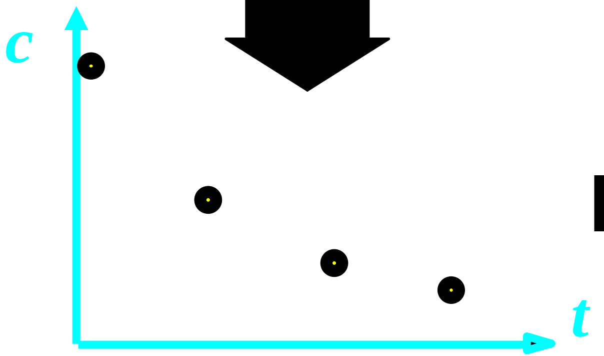
$$V\frac{dc}{dt} = W - Qc - kVc - vAc$$

accumulation = load – outflow – reaction – settling

RATE EXPERIMENT



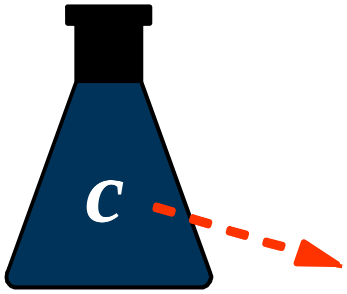
time	0	1	2	3
concentration	c_1	c_2	c_3	c_4



"rate"

k

REACTION MODEL



$c \longrightarrow$ **end products**

Mass balance: $$\frac{dc}{dt} = -kc^{n}$$

reaction "order"

reaction "rate"

REACTION ORDER

Zero-order reaction (*n* = 0)

$$\frac{dc}{dt} = -k$$

where k = zero-order reaction rate [(mg/L)/d]

First-order reaction (*n* = 1)

$$\frac{dc}{dt} = -k\,c$$

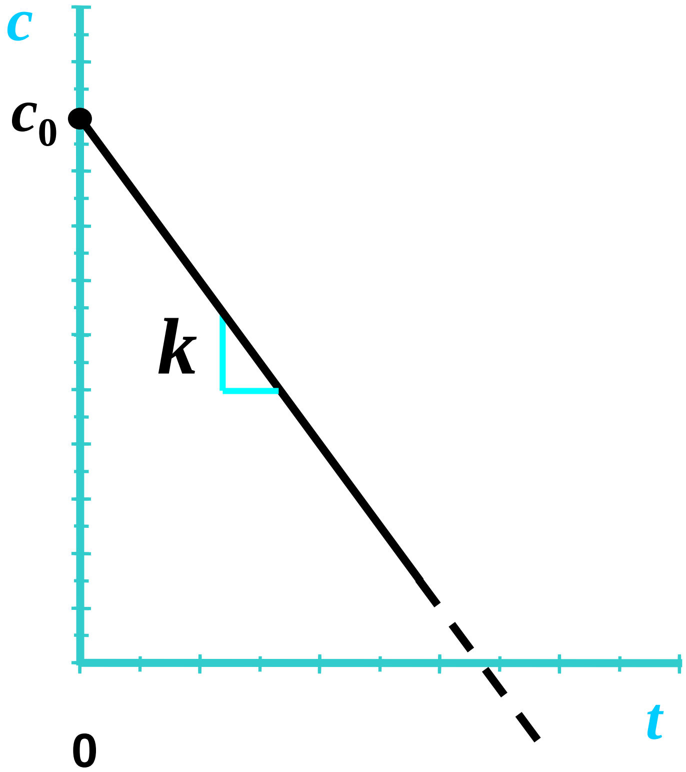
where k = first-order reaction rate [/d = per day]

ZERO-ORDER REACTION

$$\frac{dc}{dt} = -k$$

where $c = c_0$ at $t = 0$,

$$c = c_0 - kt$$



FIRST-ORDER REACTION

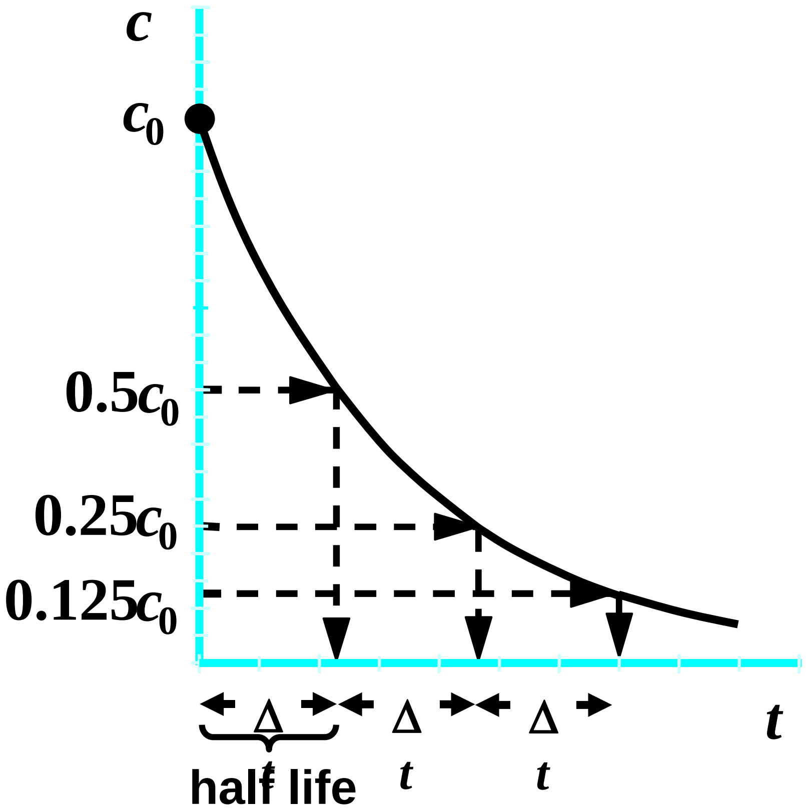
$$\frac{dc}{dt} = -kc$$

where $c = c_0$ at $t = 0$

$$c = c_0 e^{-kt}$$

FIRST-ORDER REACTIONS

$$c = c_0 e^{-kt}$$



THE "MEANING" OF A FIRST-ORDER RATE COEFFICIENT

If its magnitude is less than 0.5, *k* can be interpreted as the fraction of the pollutant that is lost per unit time.

0.25/d $\longrightarrow$ 25%/d

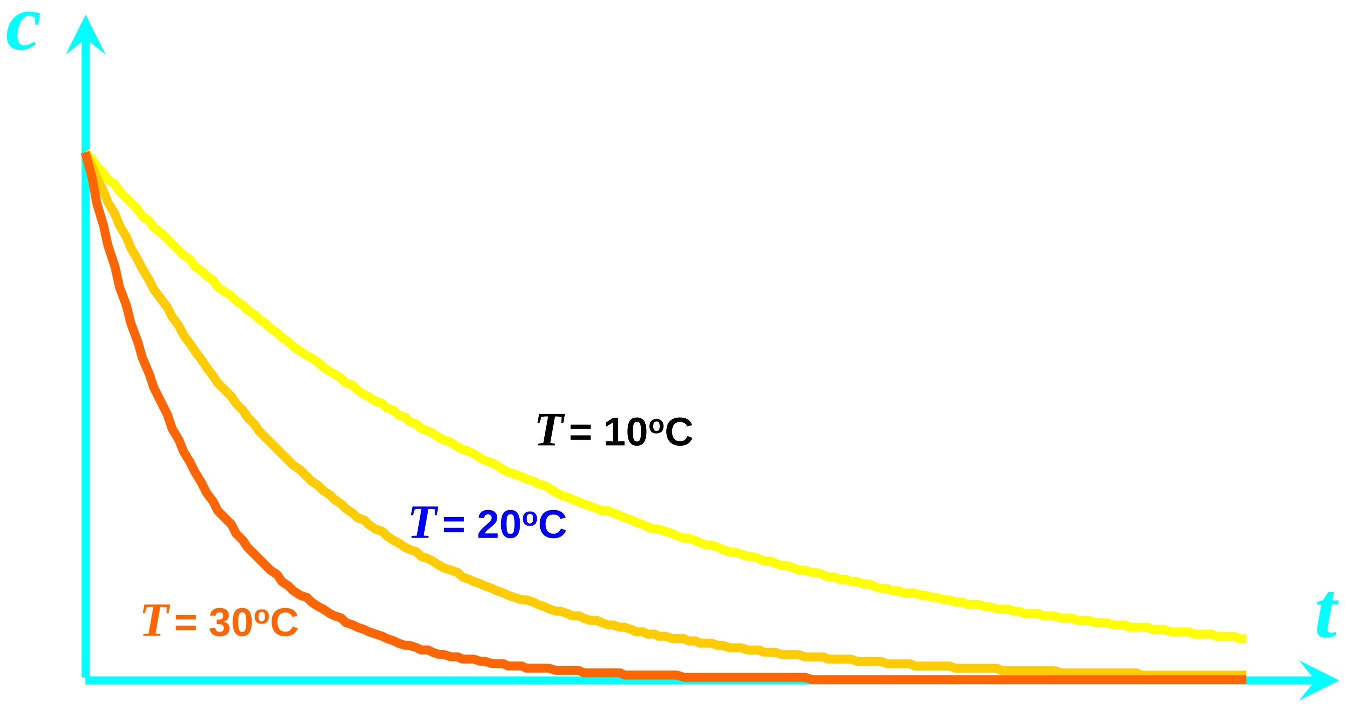
0.1/yr $\longrightarrow$ 10%/yr

2.4/d $\longrightarrow$ 240%/d ???

change units so < 0.5

$$\frac{2.4}{\cancel{d}}\ \frac{\cancel{d}}{24\ hr} = 0.1/hr \longrightarrow 10\%/hr$$

TEMPERATURE EFFECTS



TEMPERATURE EFFECTS

$$\frac{k(T_2)}{k(T_1)} = \theta^{T_2 - T_1}$$

Reference temperature

Chemical engineering: 25°C

Environmental engineering: 20°C

$$k(T) = k(20)\,\theta^{T-20}$$

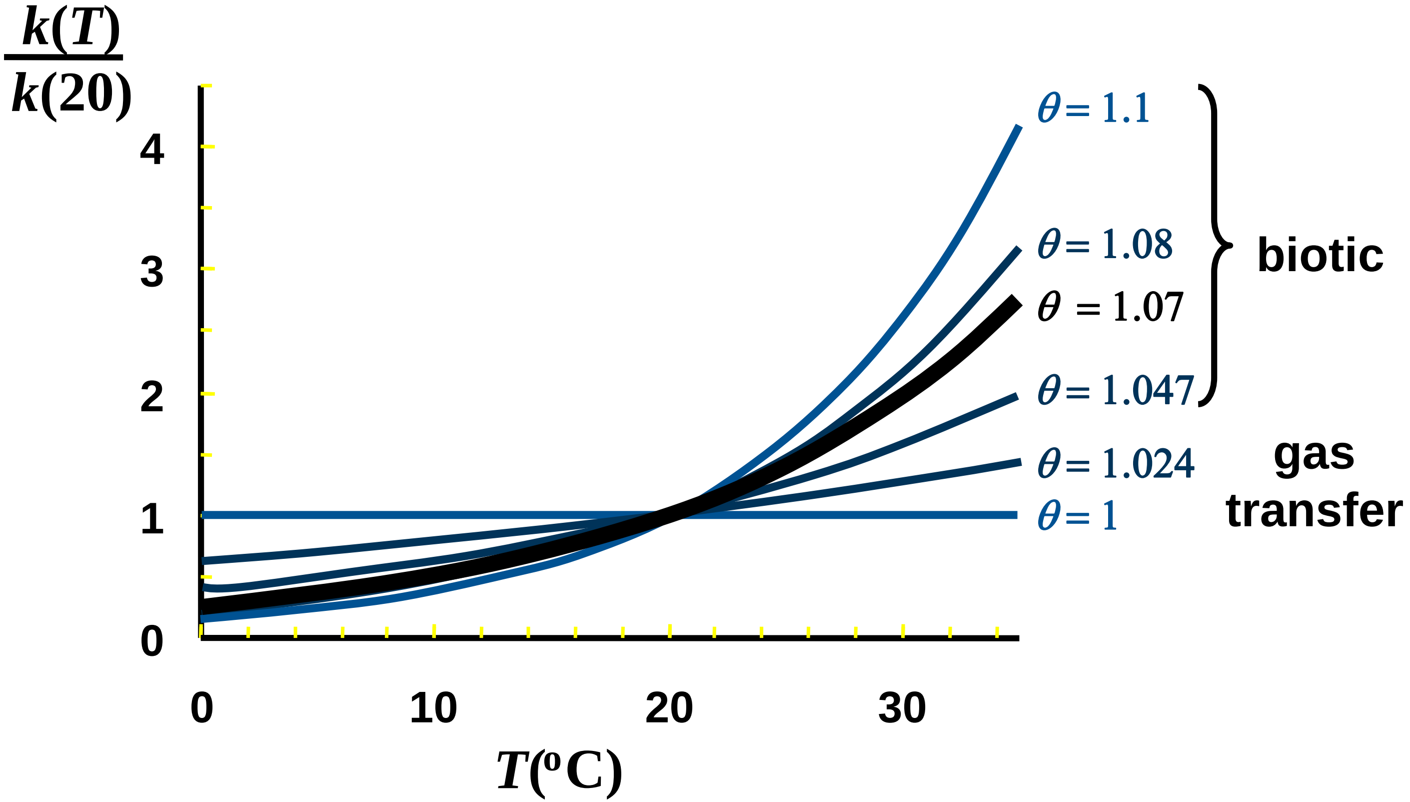
Q_{10}

- ***Used widely by biologists***
- ***How much the rate changes per 10 ºC rise in temperature***

$$Q_{10} = \frac{k(20)}{k(10)} = \theta^{10}$$

θ	Q_{10}	Reaction
1.024	1.27	Oxygen reaeration
1.047	1.58	BOD decomposition
1.066	1.89	Phytoplankton growth
1.07	**2**	**Biological "rule of thumb"**
1.08	2.16	Sediment oxygen demand

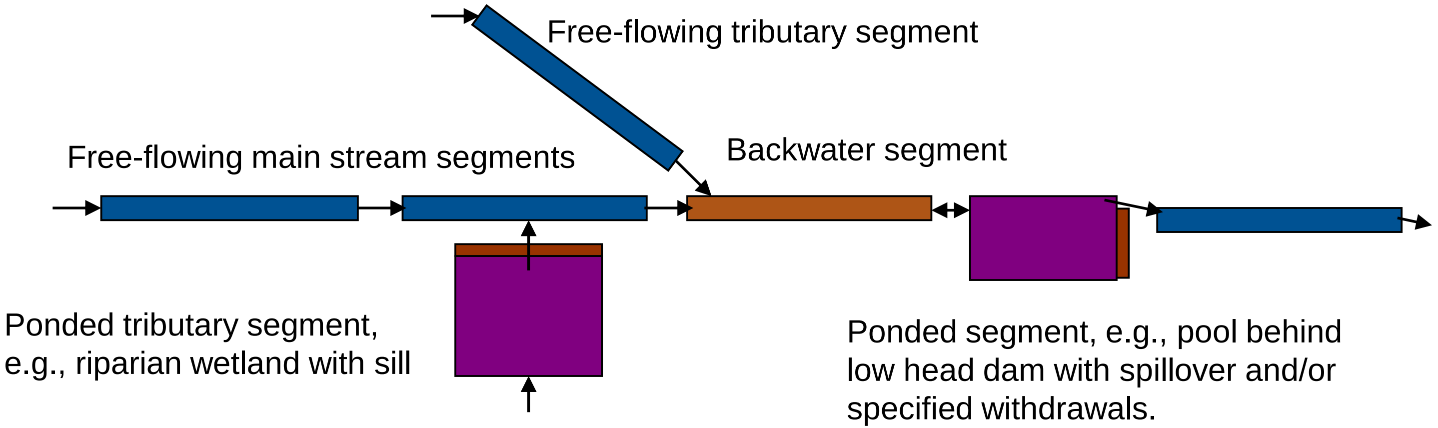
TEMPERATURE EFFECT ON THE REACTION RATE



P3. Application

- ***0-D, 1-D, 2-D, 3-D***
- ***Water Quality Problems***
- ***WQ modelling application under climate change***

0-D, 1-D, 2-D, 3-D



WASP internally calculates flows, volumes, depths, widths in: free-flowing reaches (kinematic wave eq.), ponded reaches (weir overflow eq.), and backwater reaches (dynamic flow eq's.)

Water Quality Problems

- Conventional Water Quality: DO, Eutrophication, Temperature
- Other WQ: Organic Chemicals, Nano Materials, Simple Metals, Mercury, Pathogen



Water quality under climate change

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Environmental Science & Technology

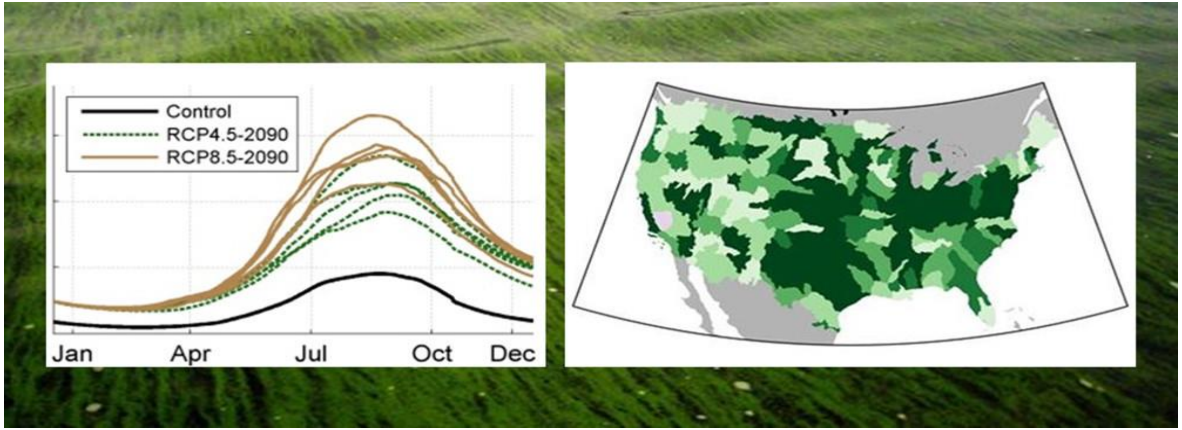
ACS AuthorChoice

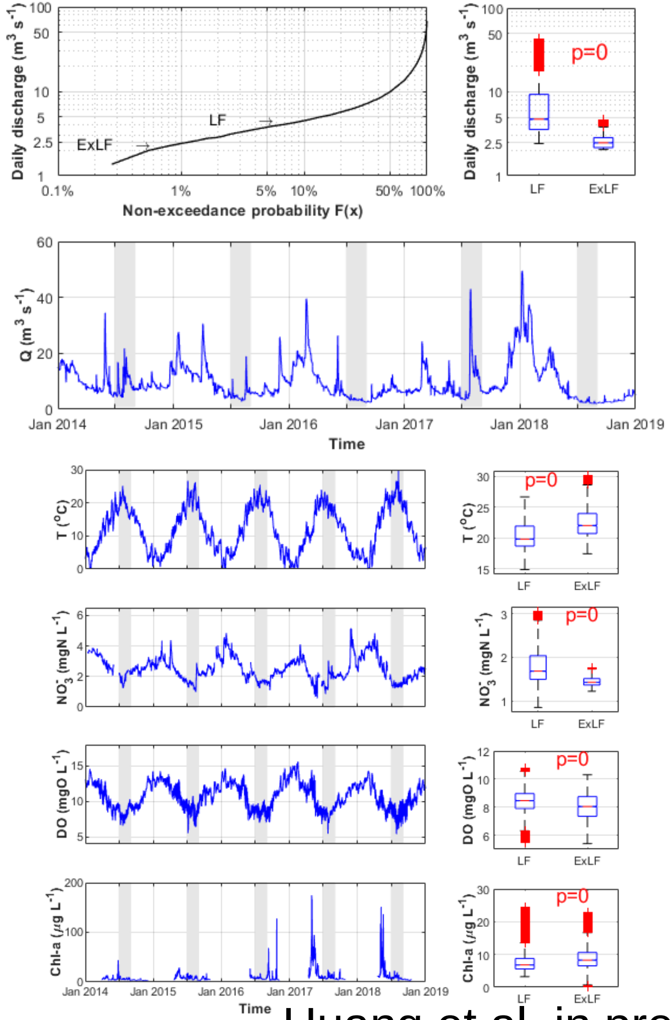
Article

pubs.acs.org/est

Climate Change Impacts on Harmful Algal Blooms in U.S. Freshwaters: A Screening-Level Assessment

Steven C. Chapra,[†] Brent Boehlert,[*,‡,§] Charles Fant,[‡] Victor J. Bierman, Jr.,[∥] Jim Henderson,[⊥] David Mills,[#] Diane M. L. Mas,[∇] Lisa Rennels,[‡] Lesley Jantarasami,[○] Jeremy Martinich,[○] Kenneth M. Strzepek,[§] and Hans W. Paerl[∞]





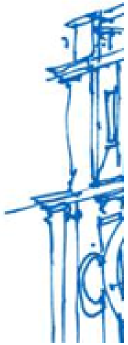
Huang et al. in prep.

Flash flood-WQ modelling application

Modelling risks of infection from post-flood ponds exemplified by cholera in Alajo neighborhood, Accra, Ghana.

Study Project
Carolina Iwane Hotta

Supervisors:
Dr. Ing. Jingshui Huang
Dr. phil. Jorge Eduardo Teixeira Leandro
Prof. Divine Kwaku Ahadzie



Objective

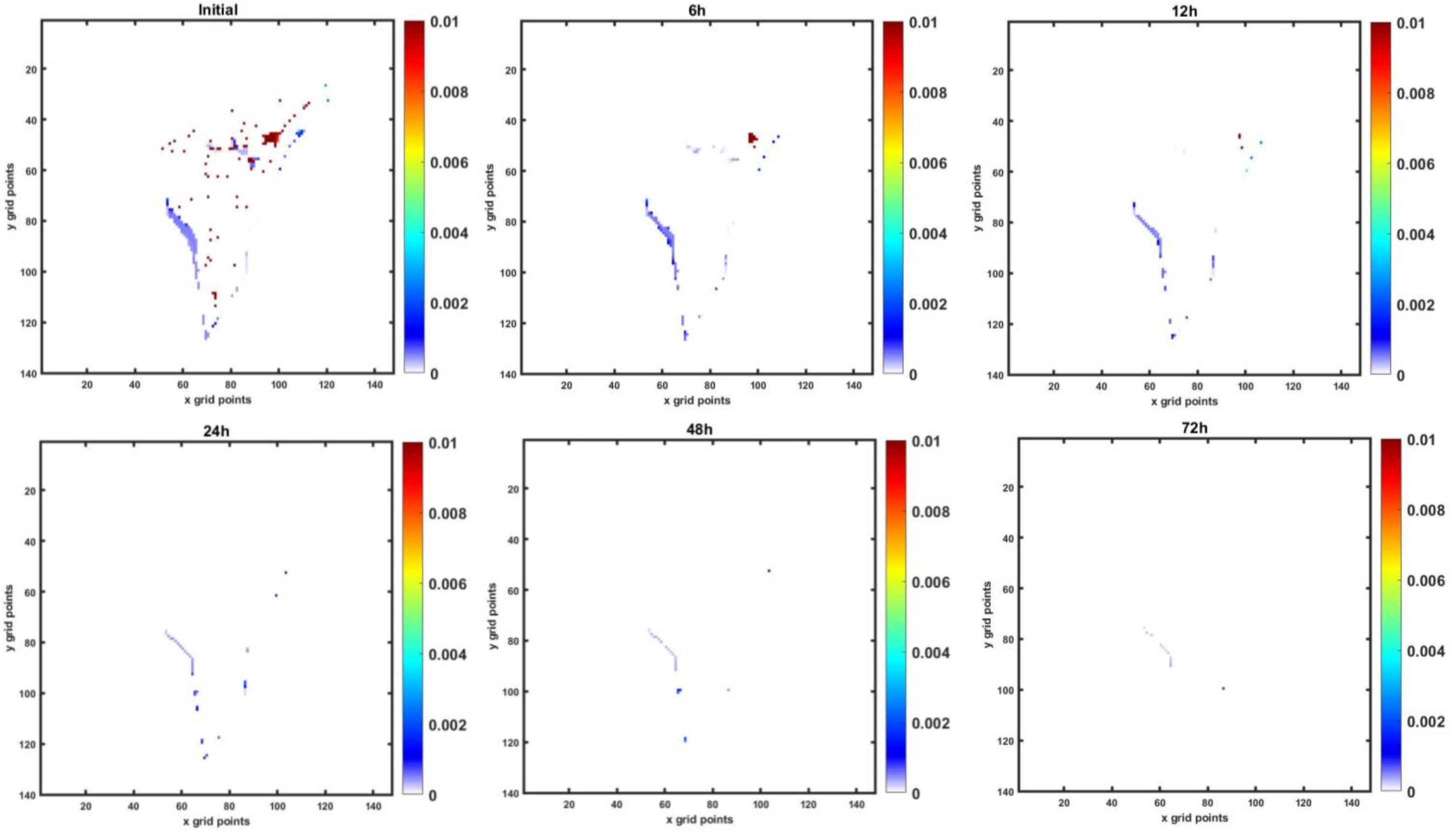
Introduction

https://www.bbc.com/pidgin/tori-47933002

Simulate the risk for the population in Alajo, Accra, of getting infected by the bacterium *Vibrio cholerae* after possible exposure to post-flood ponds.

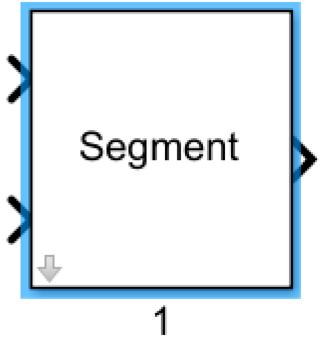
Risk of Infection after flooding

Results

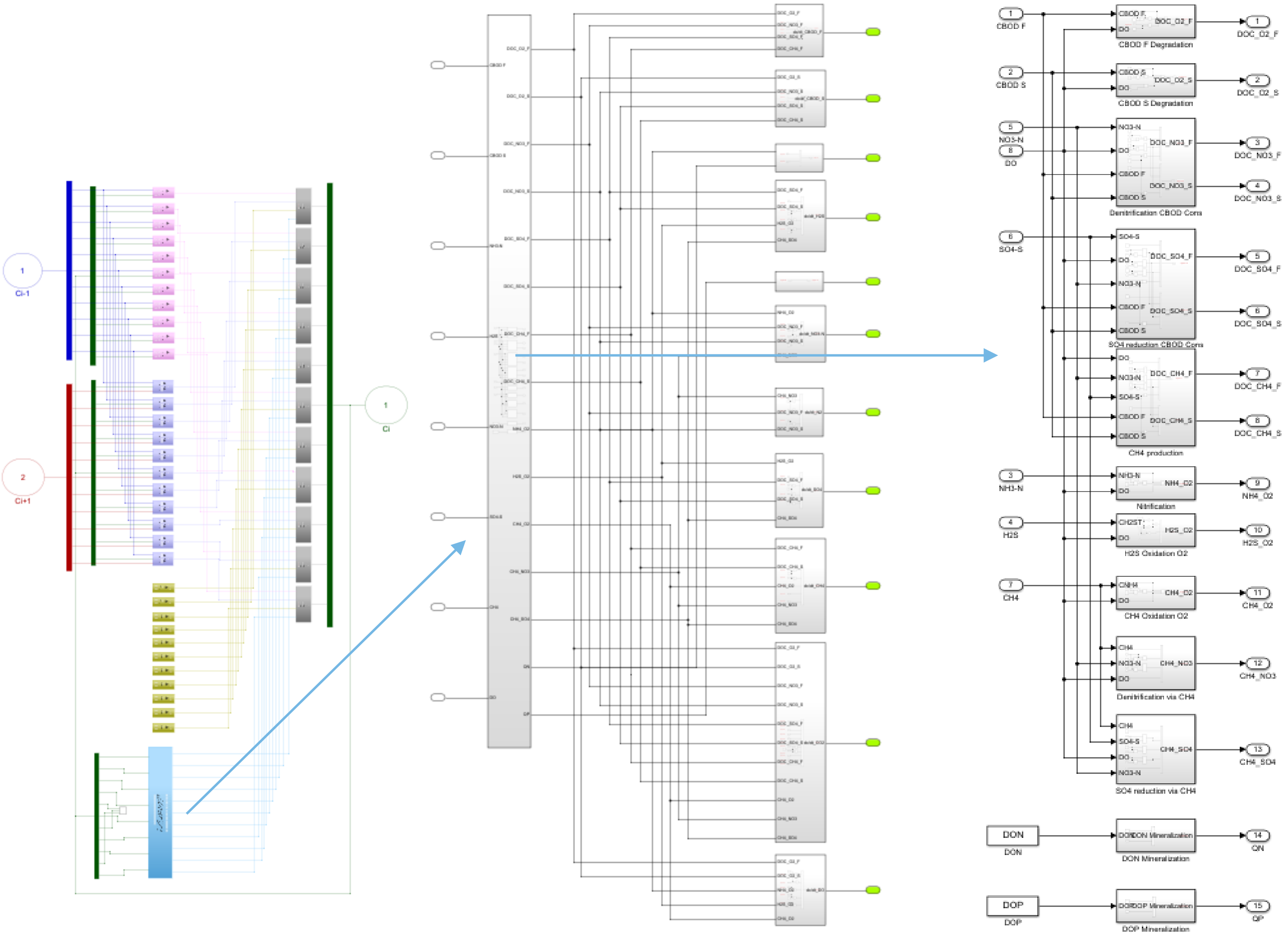


Small children swimming and/or playing in floodwater

SimShui



Segment
1



CBOD F Degradation
CBOD S Degradation
CH4 production
Nitrification
H2S Oxidation O2
CH4 Oxidation O2
Denitrification via CH4
SO4 reduction via CH4
DON Mineralization
DOP Mineralization

Cup
Cup
Segment
1
2
3
4
5
6
7
8
9
10
Cup_D
Cup_D
11
12
13
14
15
16
17
18
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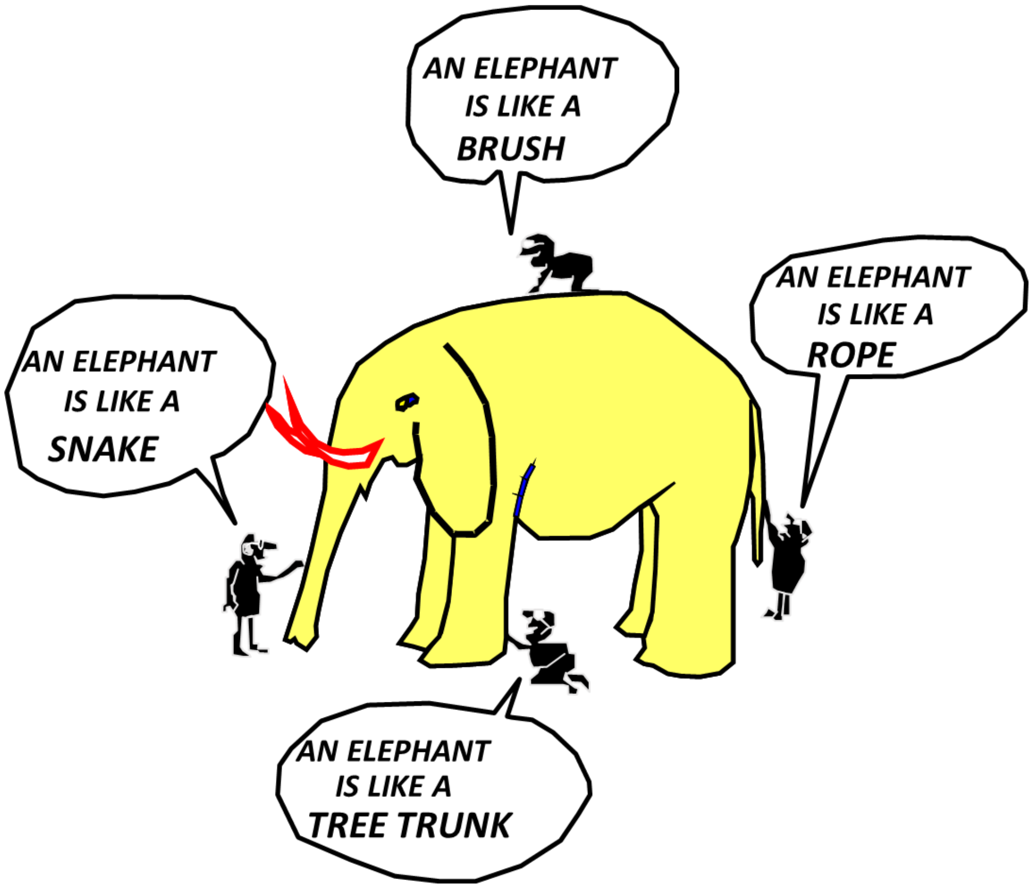
40
41
42
43
44
45
simout
Fmax for 45 segment

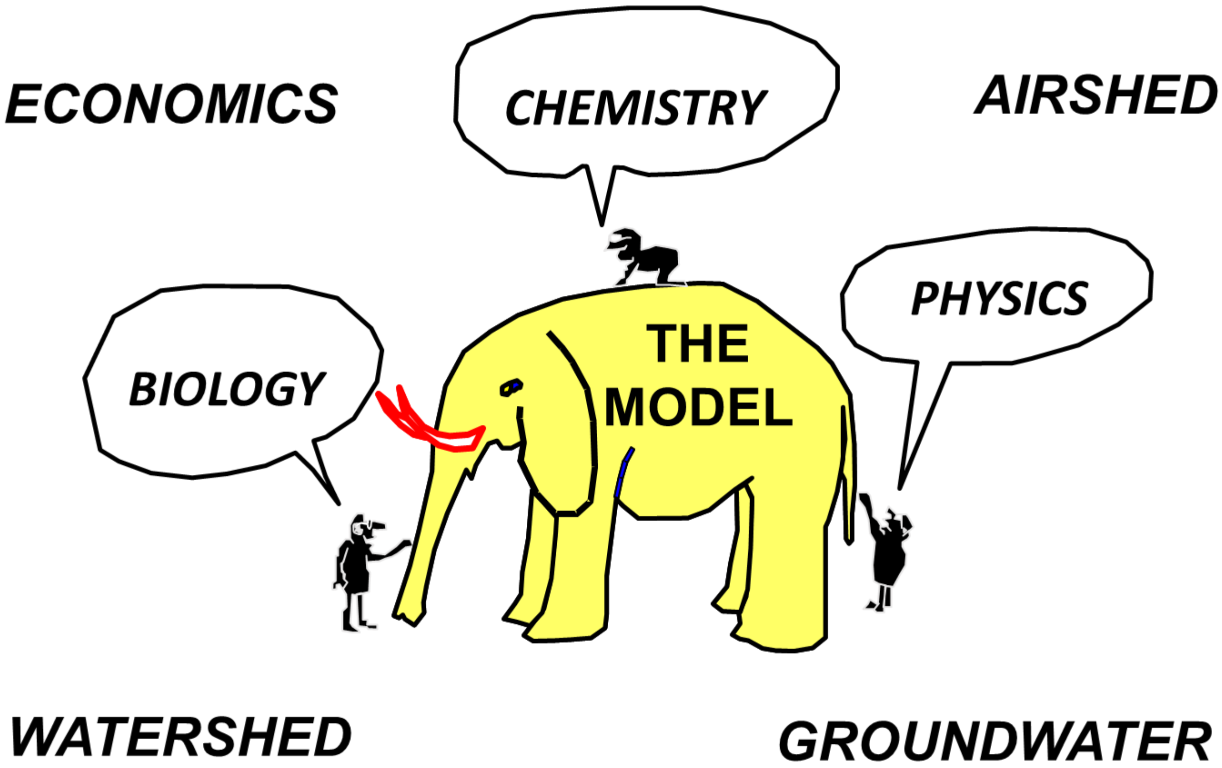
Summary

1. Introduction to Water Quality Modeling
   - What is water quality modeling?
   - Mass balance
   - Analytical & numerical solutions
2. Kinetics
   - Zero & first-order reactions
   - Temperature effects
3. Not only water quantity, but also quality!

MODELS GIVE YOU THE BIG PICTURE



THE COMPUTER MODEL TIES EVERYTHING TOGETHER



Thank you very much!

TRITON

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