Surface Water Quality Modeling



C. D. Guzman, PhD Week 1 Wednesday, Jan 22, 2020











PART 1: COMPLETELY MIXED SYSTEMS

This section is devoted to modeling well-mixed systems, including an overview of analytical and computer-oriented solution techniques and an introduction to reaction kinetics.

Analytical approach: Linear models

Computer-oriented approaches: More complex systems





Mass and Concentration

The amount of pollutant in a system is represented by its mass. Such a property is an extensive property (e.g. heat, volume, also) and is additive.

Intensive properties are normalized by a measure of system size :

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

m = mass (M) and V = volume (L³), ratio representing "strength" of pollution

Concentration is conveniently expressed in metric units. $1 \times 10^3 mg = 1 g = 1 \times 10^{-3} kg$

$$\frac{mg}{L} \frac{10^3 L}{m^3} \frac{g}{10^3 mg} = \frac{g}{m^3}$$

Prefixes

SI (International System of Unites) prefixes commonly used in water-quality modeling

Prefix	Symbol	Value
kilo-	k	10 ³
hecto-	h	10 ²
deci-	d	10-1
centi-	С	10-2
milli-	m	10-3
micro-	μ	10 ⁻⁶
nano-	n	10 ⁻⁹

Mass and Concentration

This situation is further complicated because for the dilute aqueous solutions common in most surface waters, concentration is expressed on a mass basis.

$$\frac{g}{m^3} = \frac{g}{m^3 \times (1 \, g/cm^3)} \frac{m^3}{10^6 cm^3} = \frac{g}{10^6 g} = 1 \, ppm$$

ppm stands for "parts per million"

TABLE 1.2Some water-quality variables along with typical units

Variables	Units
Total dissolved solids, salinity	$g L^{-1} \Leftrightarrow kg m^{-3} \Leftrightarrow ppt$
Oxygen, BOD, nitrogen	$\text{mg } L^{-1} \Leftrightarrow \text{g } m^{-3} \Leftrightarrow \text{ppm}$
Phosphorus, chlorophyll a, toxics	μ g L ⁻¹ \Leftrightarrow mg m ⁻³ \Leftrightarrow ppb
Toxics	ng L ⁻¹ \Leftrightarrow μ g m ⁻³ \Leftrightarrow pptr

EXAMPLE 1.1. MASS AND CONCENTRATION. If 2×10^{-6} lb of salt is introduced into 1 m³ of distilled water, what is the resulting concentration in ppb?



Rates

Properties that are normalized to time are commonly referred to as rates.

Mass loading rates describe the mass of a pollutant m which is determined over a time period t:

$$W = \frac{m}{t}$$

 $t_0, \dots, t_1, \dots, t_2, \dots, t_n$

Rates





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FIGURE 1.3

Three fundamental rates used extensively in water-quality modeling.





EXAMPLE 1.2. LOADING AND FLUX. A pond having constant volume and no outlet has a surface area A_s of 10^4 m² and a mean depth *H* of 2 m. It initially has a concentration of 0.8 ppm. Two days later a measurement indicates that the concentration has risen to 1.5 ppm. (*a*) What was the mass loading rate during this time? (*b*) If you hypothesize that the only possible source of this pollutant was from the atmosphere, estimate the flux that occurred.



Mathematical Models c=f(W)

A mathematical model is an idealized formulation that represents the response of a physical system to external stimuli. c = f(W; physics, chemistry, biology). A simple linear relationship is $c = \frac{1}{a}W$

Implementations:

1. Simulation mode. System response

2. Design mode I.

W = ac (assimilative capacity)

3. Design mode II.

$$a = \frac{W}{c}$$
 (remedial effort)

EXAMPLE 1.3. ASSIMILATION FACTOR. Lake Ontario in the early 1970s had a total phosphorus loading of approximately 10,500 mta (metric tonnes per annum, where a metric tonne equals 1000 kg) and an in-lake concentration of 21 μ g L⁻¹ (Chapra and Sonzogni 1979). In 1973 the state of New York and the province of Ontario ordered a reduction of detergent phosphate content. This action reduced loadings to 8000 mta.

(a) Compute the assimilation factor for Lake Ontario.

(b) What in-lake concentration would result from the detergent phosphate reduction action?

(c) If the water-quality objective is to bring in-lake levels down to 10 μ g L⁻¹, how much additional load reduction is needed?

Conservation of Mass and the Mass Balance

Empirical models (inductive, data based)

Mechanistic models (deductive, theoretical)

Conservation of mass (mass-balance equation) $Accumulation = loading \pm transport \pm reactions$



Accumulation = loading \pm transport \pm reactions



FIGURE 1.5

A schematic representation of the loading, transport, and transformation of two substances moving through and reacting within a volume of water.

Historical Development of Water Quality Models

Early modeling work focused on urban wasteload allocation.

Seminal work by Streeter and Phelps (1925) on Ohio River



1970–1977 (biology)

Problems: eutrophication Pollutants: nutrients Systems: lakes/estuaries/streams (1D/2D/3D) Kinetics: nonlinear, feedback Solutions: numerical



1977-present (toxics)

Problems: toxics Pollutants: organics, metals Systems: sediment-water interactions/ food-chain interactions (lakes/estuaries/streams) Kinetics: linear, equilibrium Solutions: numerical and analytical



FIGURE 1.6 Four periods in the development of water-quality modeling.



FIGURE 1.7

Capital construction costs versus degree of treatment for municipal wastewater treatment. Note that most decisions relating to tertiary waste treatment presently deal with high-percent removals. Consequently a faulty decision carries a much higher economic penalty today than in earlier years when primary and secondary waste treatment were dominant.

Overview of the book

Part I Completely Mixed Systems Part II Incompletely Mixed Systems Part III Water Quality Environments Part IV Dissolved oxygen and bacteria Part V Eutrophication Part VII Toxic substance modeling