"Mass Balance"

Module 1: Basic Concepts, Lecture 1

Chemical Fate and Transport in the Environment, 2nd edition. H.F. Hemond and E.J. Fechner-Levy. Academic Press. London. 2000.



The Start of the Problem

"By sensible definition any by-product of a chemical operation for which there is no profitable use is a waste. The most convenient, least expensive way of disposing of said waste – up the chimney or down the river – is the best."

Haynes, W. American Chemical Industry, A History. Van Nostrand, NY. 1954.

Common Mathematical Basis for Predicting Movement of Pollutants

- The mathematics describing physical transport in each medium are almost identical.
- The transport equation that models the mixing of industrial effluent into a river is also useful for describing the movement of contaminants in groundwater or the mixing of air pollutants in the atmosphere.

Common Principles

• Knowledge of the principles underlying the fate and transport of chemicals in the environment allows problems ranging from local to global scales to be defined and analyzed.

Other Commonly Used Concentration Expressions for Water

- Molarity, M: number of moles per L of solution. A mole (mol) contains 6.23 x 10²³ atoms (or molecules) of the substance, and is the weight (in grams) equal to the MW of the substance (a "gram molecular weight").
- Normality, N: number of equilivents per L of water. If a chemical has 2 electronic charge units per molecule, 1 mol of the chemical constitutes 2 equilivents: A mole of sulfate (SO₄²⁻) is equal to 2 equilivents, and a one molar (1 *M*) solution of sodium sulfate (Na₂SO₄) is two normal (2 *N*).

1.2 Chemical Concentrations

- Mass per unit volume [M/L³], such as mg/L, is the most common expression for water.
- When describing mass, important to specify which chemical species is being expressed (such as when expressing phosphate in mg/L as P, or mg/L as PO₄, the range in concentration would be MW = 17 vs. MW = 17 + 4(16) = 81, or a ratio of 4.76 x).
- ppm, or ppb, are usually less accurate units than mg/L or μg/L in water, but commonly used in air or soil, where concentrations are frequently expressed as mass per unit mass [M/M], such as mg pollutant/kg soil.

Soil and Air Contaminant Concentration Expressions

- Chemical concentrations in soil (and sediment) are usually best expressed as [M/M], as the volume of soil is highly variable due to compaction. Units are usually expressed as mg pollutant/kg soil.
- Chemical concentrations in air are similar, as the air is highly compressible and the volume can undergo rapid and large changes.

1.3 Mass Balances and Units

- Calculating chemical mass balances is the most important and basic step in analyzing environmental fates of discharged chemicals.
- Control volumes are described around a location of interest and conservation of mass is applied to that volume. Equations are developed and can be solved to determine the concentrations of the contaminant in the control volume, considering inputs and outputs across the control volume boundary.



Mass Balance Equations

• Mass balance equation for a control volume for any time interval:

Change in storage of mass = mass transported in – mass transported out + mass produced by sources – mass eliminated by sinks

Mass Balance Rate Equation

 Mass balance equation can also be written in terms of rates (mass per time, or [M/T]):

Rate of change in storage of mass = mass transported rate in – mass transport rate out + mass production rate by sources – mass elimination rate by sinks













MASS IN = MASS OUT
M1 + M2 = M3 + M4
M1 = Q1P1, CSO tracer mass,
M2 = Q2P2, Fresh Creek leakage tracer mass,
M3 = Q3P3, pumpback tracer mass, and
M4 = 94P4, discharge to Fresh Creek tracer mass.
Q1 = Total volume of CSO flowing into
the FBM for the event
92 = Volume of Fresh Creek leakage into the FBM
Q3 = Total volume of pumpback to treatment plant
P1 = CSO tracer concentration
P2 = Fresh Creek tracer concentration
P3 = Pumpback tracer concentration
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CS	SO Volur	ne (mill	lions of ga	llons):
0.26	6.8		16	
Q1 1.00	Q1	1.00	Q1	1.00
P3 0.30	P1	0.51	P1	0.78
Q3 0.23	P3	0.29	P2	0.35
P3XQ10.16	Q3	0.22	P3	0.30
93X91 0.12	P2	0.20	93	0.23
	P3XQ1	0.15	P3XQ1	0.16
1	93X91	0.12		
Q1 (CSO dischar	ge volu	ne)		
3 (pumpback v	olume)			
P1 (CSO specific	conduc	tivity)		
2 (Fresh Creek	specific	condu	ctivity)	
P3 (numphack s	necific c	onduct	ivity)	

