Updated: 7 September 2017

Print version

CEE 577: Surface Water Quality Modeling

Lecture #2

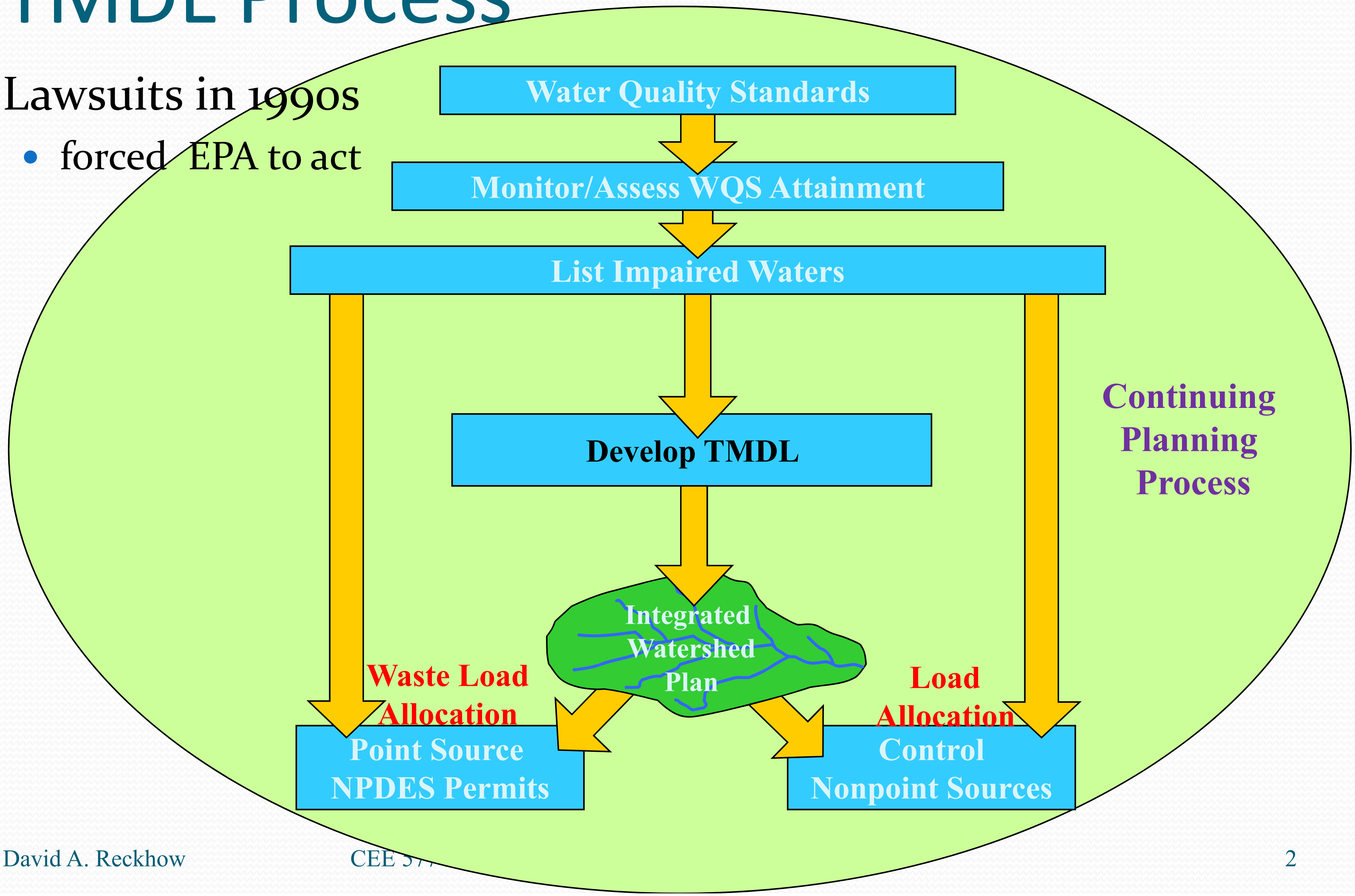
(modeling fundamentals & mass balance)

Chapra, L1

(pp. 3-20)

TMDL Process

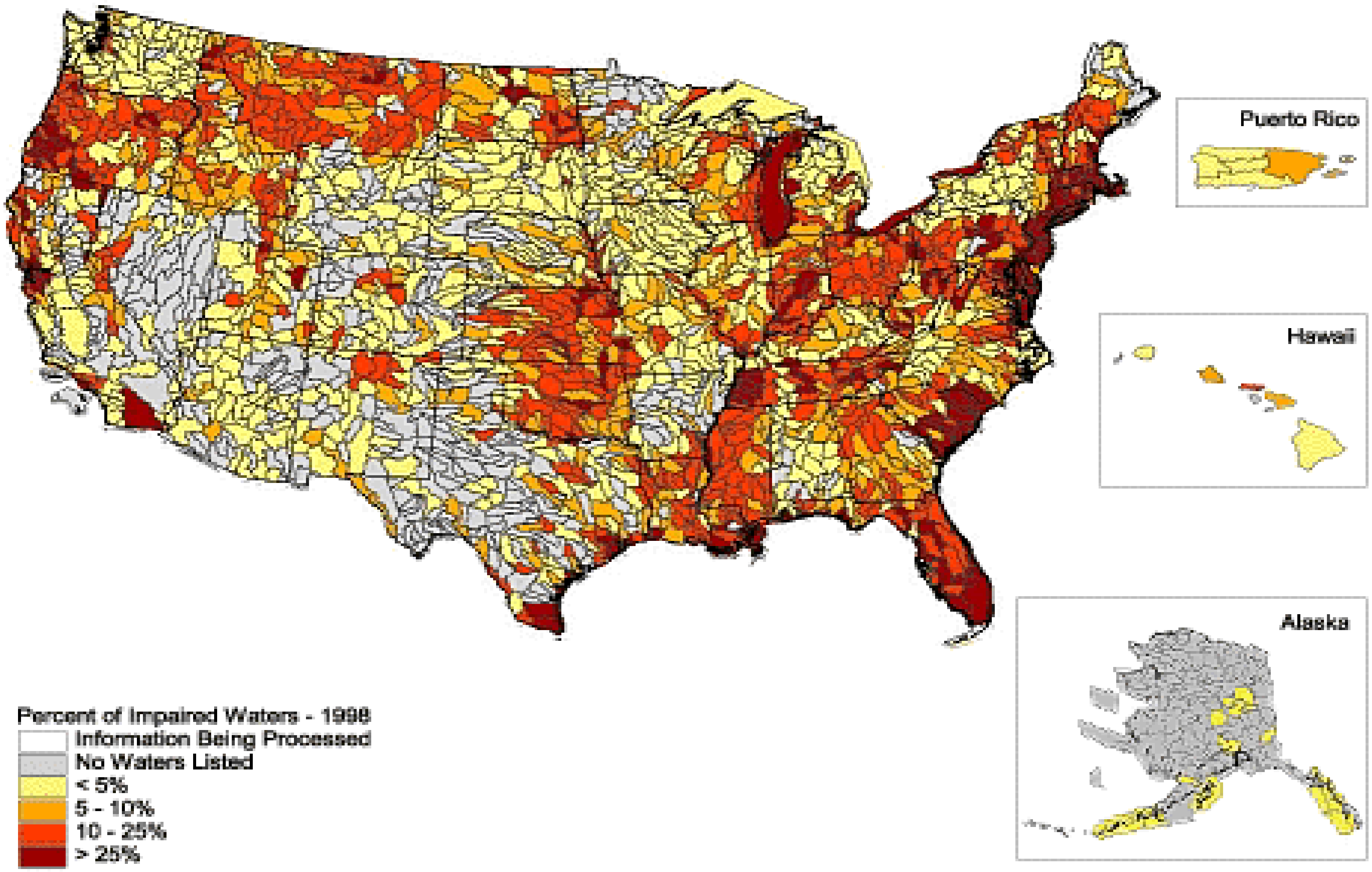
- Lawsuits in 1990s
  - forced EPA to act



Top 10 Categories of Impairment Identified on the 1998 303d lists

Cause of Impairment	Count
Sediments	6133
Pathogens	5281
Nutrients	4773
Metals	3984
Dissolved Oxygen	3758
Other Habitat Alterations	2106
Temperature	1884
Ph	1798
Impaired Biologic Community	1440
Pesticides	1432

Impaired Watersheds in US



See: <u>EPA's impaired waters page</u>

Impaired waters by state

State	Number	State	Number	State	Number
Alabama	209	Kentucky	1,300	North Dakota	214
Alaska	35	Louisiana	250	Ohio	267
Arizona	84	Maine	114	Oklahoma	743
Arkansas	224	Maryland	184	Oregon	1,397
California	691	Massachusetts	837	Pennsylvania	6,957
Colorado	244	Michigan	2,352	Puerto Rico	165
Connecticut	425	Minnesota	1,144	Rhode Island	162
Delaware	101	Mississippi	180	South Carolina	961
DC	36	Missouri	245	South Dakota	159
Florida	2,292	Montana	604	Tennessee	1,028
Georgia	215	Nebraska	260	Texas	651
Guam	47	Nevada	181	Utah	118
Hawaii	309	NH	1,449	Vermont	126
Idaho	915	New Jersey	745	Virginia	1,523
Illinois	1,057	New Mexico	196	Washington	2,419
Indiana	1,836	New York	528	West Virginia	1,097
Iowa	474	North Carolina	1,270	Wisconsin	59
Kansas	1,387			Wyoming	111

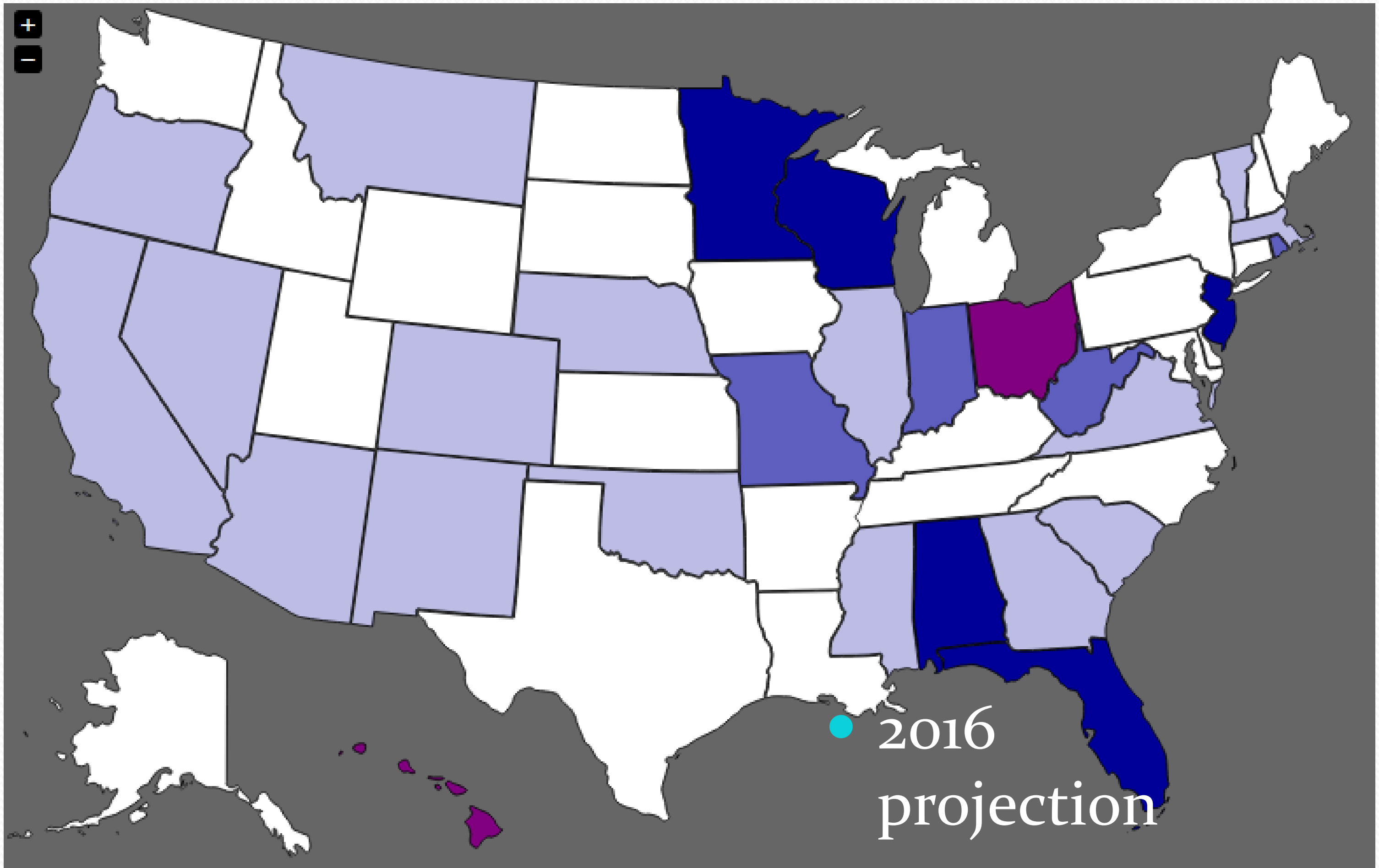
http://iaspub.epa.gov/waters10/attains_nation_cy.control?p_report_type=T; accessed 24 Jan 2012

August 2012

Progress Toward Clean Water Act Adopted Numeric Nutrient Criteria

http://www.epa.gov/nandppolicy/progress.html

Nutrient Criteria



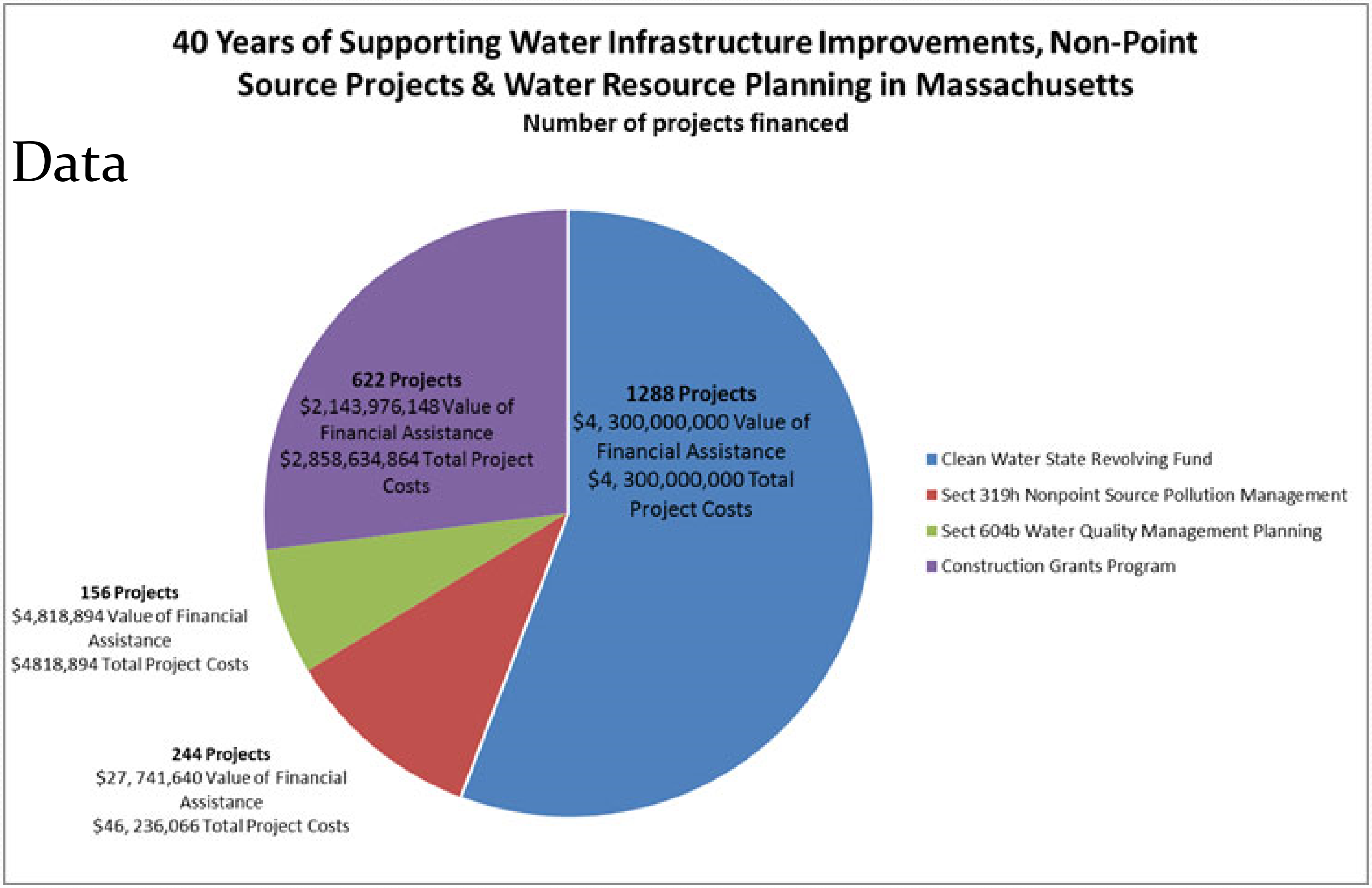
- 2016 projection

	District of Columbia
	American Samoa
	Commonwealth of Northern Marianas
	Guam
	Puerto Rico
	US Virgin Islands

Level 5	Complete set of N and P criteria for all watertypes**
Level 4	2 or more watertypes with N and/or P criteria
Level 3	1 watertype with N and/or P criteria
Level 2	Some waters with N and/or P criteria
Level 1	No N and/or P criteria

MA DEP

2013 Data



Priority Pollutants: Pg 1 of 8

	Priority Pollutant	CAS Number	Freshwater CMC (µg/L)	Freshwater CCC (µg/L)	Saltwater CMC (µg/L)	Saltwater CCC (µg/L)	Human Health; For Consumption of: Water + Organism (µg/L)	Human Health; For Consumption of: Organism Only (µg/L)	FR Cite/ Source
1	Antimony	7440360					5.6 B	640 B	65FR66443
2	Arsenic	7440382	340 A,D,K	150 A,D,K	69 A,D,bb	36 A,D,bb	0.018 C,M,S Z	0.14 C,M,S	65FR31682 57FR60848
3	Beryllium	7440417							65FR31682
4	Cadmium	7440439	2.0 D,E,K,bb	0.25 D,E,K,bb	40 D,bb	8.8 D,bb	Z		EPA-822-R-01-001 65FR31682
5a	Chromium (III)	16065831	570 D,E,K	74 D,E,K			Z Total		EPA820/B-96-001 65FR31682
5b	Chromium (VI)	18540299	16 D,K	11 D,K	1,100 D,bb	50 D,bb	Z Total		65FR31682
6	Copper	7440508	13 D,E,K,cc	9.0 D,E,K,cc	4.8 D,cc,ff	3.1 D,cc,ff	1,300 U		65FR31682
7	Lead	7439921	65 D,E,bb,gg	2.5 D,E,bb,gg	210 D,bb	8.1 D,bb			65FR31682
8a 8b	Mercury Methylmercury	7439976 22967926	1.4 D,K,hh	0.77 D,K,hh	1.8 D,ee,hh	0.94 D,ee,hh		0.3 mg/kg J	62FR42160 EPA823-R-01-001
9	Nickel	7440020	470 D,E,K	52 D,E,K	74 D,bb	8.2 D,bb	610 B	4,600 B	65FR31682
10	Selenium	7782492	L,R,T	5.0 T	290 D,bb,dd	71 D,bb,dd	170 Z	4200	62FR42160 65FR31682 65FR66443
11	Silver	7440224	3.2 D,E,G		1.9 D,G				65FR31682
12	Thallium	7440280					1.7 B	6.3 B	65FR31682

Priority Pollutants: Pg 8 of 8

- Revised Human Health Water Quality Criteria (December 31, 2003)

	Priority Pollutant	CAS Number	Freshwater CMC (µg/L)	Freshwater CCC (µg/L)	Saltwater CMC (µg/L)	Saltwater CCC (µg/L)	Human Health; For Consumption of: Water + Organism (µg/L)	Human Health; For Consumption of: Organism Only (µg/L)	FR Cite/ Source
111	Dieldrin	60571	0.24 K	0.056 K,O	0.71 G	0.0019 G,aa	0.000052 B,C	0.000054 B,C	65FR31682 65FR66443
112	alpha-Endosulfan	959988	0.22 G,Y	0.056 G,Y	0.034 G,Y	0.0087 G,Y	62 B	89 B	65FR31682 65FR66443
113	beta-Endosulfan	33213659	0.22 G,Y	0.056 G,Y	0.034 G,Y	0.0087 G,Y	62 B	89 B	65FR31682 65FR66443
114	Endosulfan Sulfate	1031078					62 B	89 B	65FR66443
115	Endrin	72208	0.086 K	0.036 K,O	0.037 G	0.0023 G,aa	0.76 B	0.81 B,H	65FR31682
116	Endrin Aldehyde	7421934					0.29 B	0.30 B,H	65FR66443
117	Heptachlor	76448	0.52 G	0.0038 G,aa	0.053 G	0.0036 G,aa	0.000079 B,C	0.000079 B,C	65FR31682 65FR66443
118	Heptachlor Epoxide	1024573	0.52 G,V	0.0038 G,V,aa	0.053 G,V	0.0036 G,V,aa	0.000039 B,C	0.000039 B,C	65FR31682 65FR66443
119	Polychlorinated Biphenyls PCBs:			0.014 N,aa		0.03 N,aa	0.000064 B,C,N	0.000064 B,C,N	65FR31682 65FR66443
120	Toxaphene	8001352	0.73	0.0002 aa	0.21	0.0002 aa	0.00028 B,C	0.00028 B,C	65FR31682 65FR66443

Non-priority Pollutants (pg 3 of 3)

	Non Priority Pollutant	CAS Number	Freshwater CMC (µg/L)	Freshwater CCC (µg/L)	Saltwater CMC (µg/L)	Saltwater CCC (µg/L)	Human Health For Consumption of: Water + Organism (µg/L)	Human Health For Consumption of: Organism Only (µg/L)	FR Cite/Source
32	Oxygen, Dissolved Freshwater Oxygen, Dissolved Saltwater	7782447	WARMWATER AND COLDWATER MATRIX -- SEE DOCUMENT N SALTWATER – SEE DOCUMENT						Gold Book EPA-822R-00-012
33	Parathion	56382	0.065 J	0.013 J					Gold Book
34	Pentachlorobenzene	608935					1.4 E	1.5 E	65FR66443
35	pH			6.5 - 9 F		6.5 - 8.5 F,K	5 - 9		Gold Book
36	Phosphorus Elemental	7723140				0.1 F,K			Gold Book
37	Nutrients		See EPA's Ecoregional criteria for Total Phosphorus, Total Nitrogen, Chlorophyll *a* and Water Clarity (Secchi depth for lakes; turbidity for streams and rivers) (& Level III Ecoregional criteria)						P
38	Solids Dissolved and Salinity	--					250,000 A		Gold Book
39	Solids Suspended and Turbidity		NARRATIVE STATEMENT -- SEE DOCUMENT F						Gold Book
40	Sulfide-Hydrogen Sulfide	7783064		2.0 F		2.0 F			Gold Book
41	Tainting Substances		NARRATIVE STATEMENT-- SEE DOCUMENT						Gold Book
42	Temperature	--	SPECIES DEPENDENT CRITERIA -- SEE DOCUMENT M						Gold Book
43	Tetrachlorobenzene,1,2,4,5-	95943					0.97 E	1.1 E	65FR66443
44	Tributyltin (TBT)	--	0.46 Q	0.063 Q	0.37 Q	0.010 Q			EPA 822-F-00-008
45	Trichlorophenol,2,4,5-	95954					1,800 B,E	3,600 B,E	65FR66443

Basis for Setting Standards

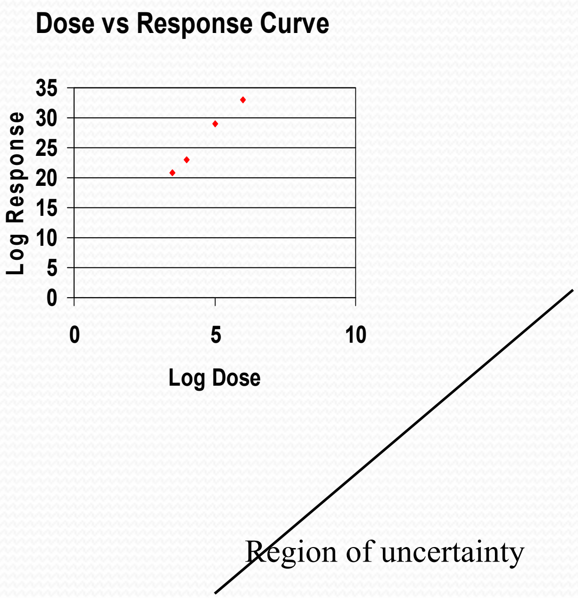
- Experimentation
  - animal testing, human exposure
- Attainability
  - economic & technical feasibility
- Established practice
- Risk Assessment

Definitions

- Risk: the probability of occurrence of adverse health effects in humans
- Risk Assessment: the process of characterizing the nature and probability of adverse health effects of human exposure to environmental hazards
- Risk Management: the process of evaluating and selecting among alternative regulatory actions

Four steps in a Risk Assessment

- Hazard Identification
  - what is it?
- Dose Response
  - see graph
- Human Exposure
  - actual doses and routes
- Risk Characterization



Comparative Risks

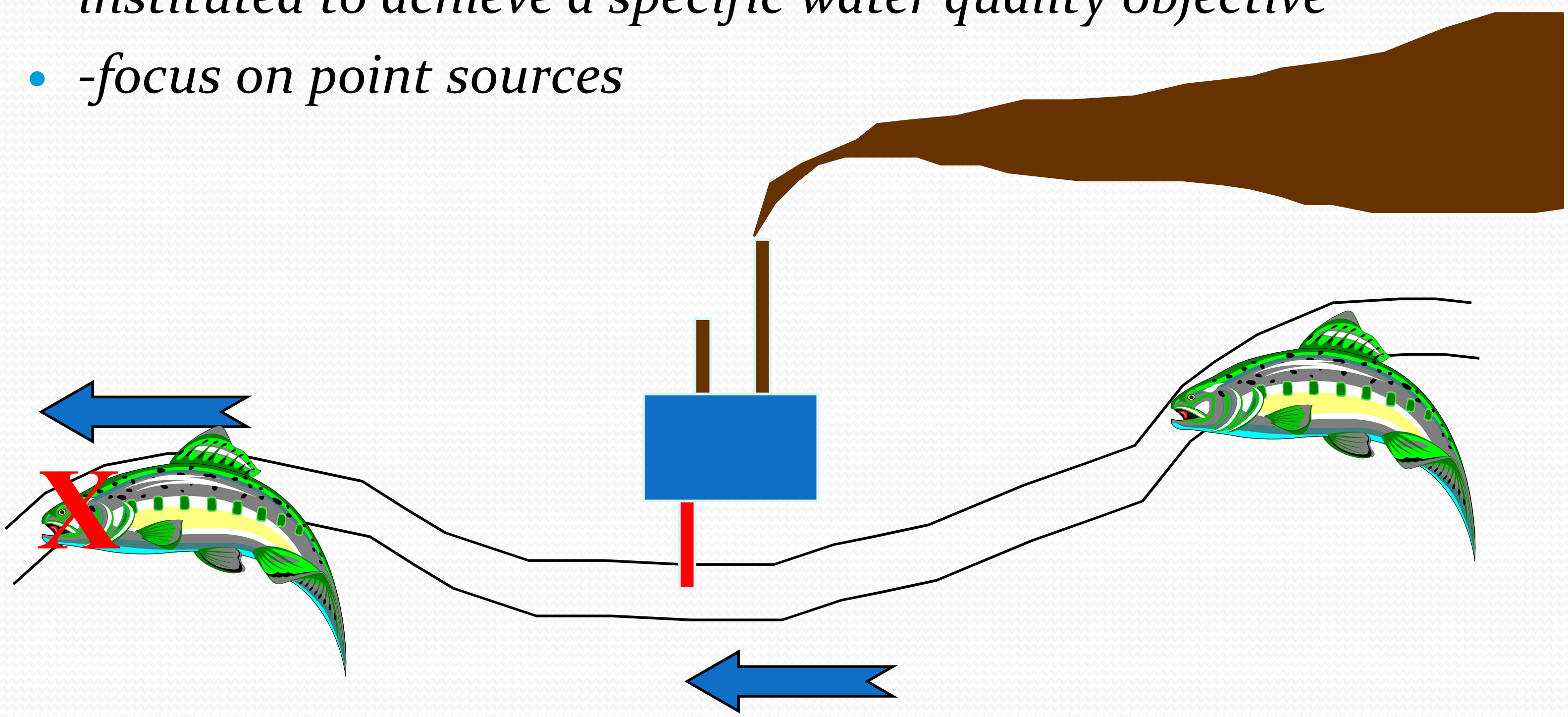
All increase chance of death in any year by 0.000001

Activity	Cause of Death
Smoking 1.4 cigarettes	Cancer, heart disease
Spending 1 hr. in a coal mine	Black lung disease
Living 2 days in NYC or Boston	Air pollution
Living 2 months in Denver	Cancer caused by cosmic radiation
One chest X-ray	Cancer caused by radiation
Eating 40 tbs. of peanut butter	Liver cancer caused by Aflatoxin B
Drinking 30 12-oz. cans of diet soda	Cancer caused by saccharin
Living 150 yrs. within 20 miles of a nuclear power plant	Cancer caused by radiation

See: Science article on value assigned to human life

Water Quality Modeling Objectives

- Waste Load Allocation
  - *-to determine the environmental controls that must be instituted to achieve a specific water quality objective*
  - *-focus on point sources*



Evolution of municipal systems

- Safe water supply
  - Need recognized by studies such as John Snow's
- Wastewater Collection
  - First just removal
  - Then need for treatment
    - Later quantified in WLA

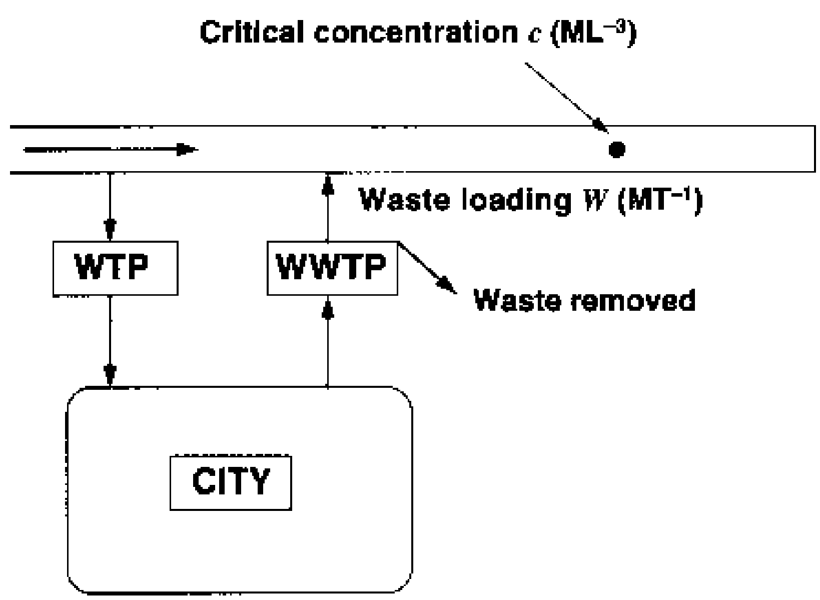


Figure 1.1 from Chapra, 1997

Objectives (cont.)

- TMDL – total maximum daily load
  - *The more general process of waste load assessment and control in a watershed*
  - *Encompassing point sources (WLA) and non-point sources (LA)*

Water Quality Management

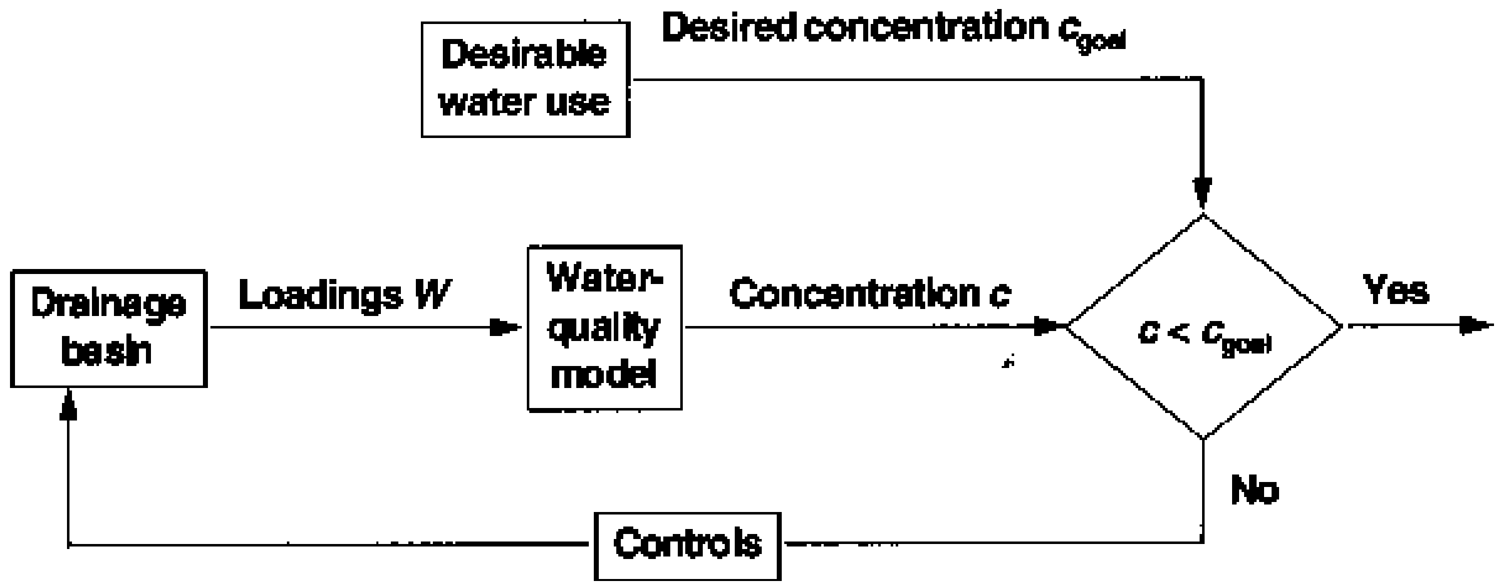


Figure 1.2 from Chapra, 1997

Objectives (cont.)

- Toxics Modeling
  - *to understand the fate of hazardous substances in the aquatic environment*
- General Understanding of the Ecosystem
  - *to understand the response of natural system to pollutant inputs*
- Errors?

TABLE 1.1 PRINCIPAL POLLUTION PROBLEMS, AFFECTED USES, AND ASSOCIATED WATER QUALITY VARIABLES (From Thomann & Mueller, 1987)

Manifestation of problem	Water use interference	Water quality problem	Water quality variables
1 Fish kills Nuisance odors, H_2S "Nuisance" organisms Radical change in ecosystem	Fishery Recreation Ecological health	Low DO (dissolved oxygen)	BOD NH_3, org N, Organic solids Phytoplankton, DO
2 Disease transmission Gastrointestinal disturbance, eye irritation	Water supply, Recreation	High bacterial levels	Total coliform bacteria, Fecal coliform bacteria, Fecal streptococci, Viruses
3 Tastes and odors-blue green algae Aesthetic beach nuisances, algal mats "Pea soup" Unbalanced ecosystem	Water supply, Recreation, Ecological health	Excessive plant growth, (Eutrophication)	Nitrogen, Phosphorus, Phytoplankton
4. Carcinogens in water supply Fishery closed-unsafe toxic levels, Ecosystem upset; mortality, reproductive impairment	Water supply Fishery Ecological health	High toxic chemical levels	Metals Radioactive substances Pesticides Herbicides Toxic product chemicals

Rates

- Determination of Mass Loading
  - Point Sources - General Concepts

$$W(t) = Q(t) \bullet c(t)$$

    - Important Conversion Factors

$$8.34 \frac{lb \bullet liters}{mg \bullet MG} \quad 2.45 \frac{Kg \bullet liters \bullet \sec}{mg \bullet ft^3 \bullet day} \quad 5.39 \frac{lb \bullet liters \bullet \sec}{mg \bullet ft^3 \bullet day}$$

Rates (cont.)

$U \equiv$ velocity of water

$A_c \equiv$ cross-sectional area

- Related Rates
  - Volumetric flow rate

$$Q = UA_c$$

  - Mass Flux rate

$$J = \frac{m}{tA_c} = \frac{W}{A_c} = Uc$$

Refer to Example 1.2 (pg 9)

And therefore, $W = JA_c$

Model Implementations

- The Model
  - concentration, c, is proportional to loading, W, by the reciprocal of an assimilation factor, a
- Simulation Mode
  - $c=W/a$
- Design Mode I Assimilative Capacity
  - $W=ac$
- Design Mode II Environmental Modification
  - $a=W/c$

Two Approaches to Modeling

- Empirical Modeling
  - based on inductive approach
  - heavily dependent on **statistical analysis** of existing data
- Mechanistic Modeling
  - based on deductive approach
  - more dependent on **theory** of underlying processes
  - emphasized in Chapra's book

Mass Balance or Mass Inventory

- Also known as conservation of mass
  - Key to mechanistic WQ modeling

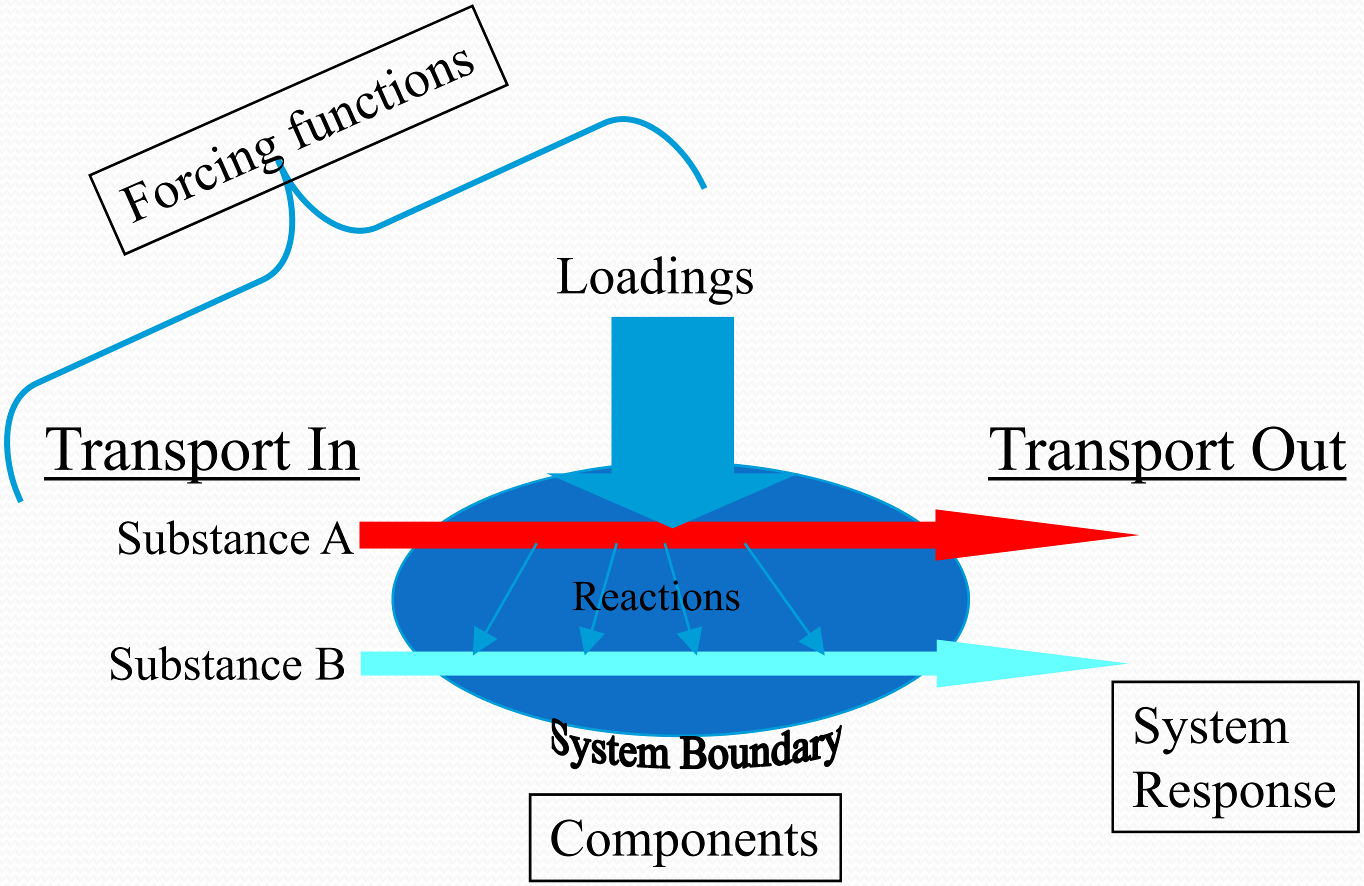
$$Accumulation = loadings \pm transport \pm reactions$$

  - If sources are in balance with sinks, mass remains constant and we are at steady state:

$$Accumulation = 0$$

  - Separate mass balances written for each substance

Typical Mechanistic Model



Based on: Figure 1.5 from Chapra, 1997

Spatial/Temporal Resolution

- When spatial or temporal concentration differences are important, system may be divided into sub-volumes or times
  - Segmentation is the process of dividing space and matter into increments
    - space: 1, 2 or 3 dimensions
  - Resolution is the degree to which space, time and matter are segmented

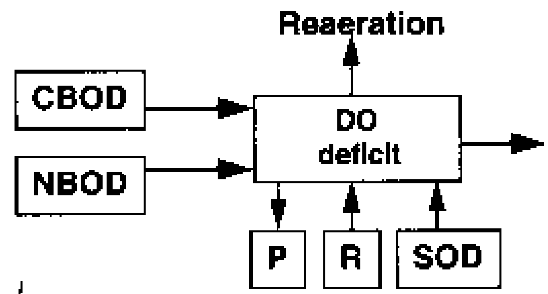
Historical Development of Mechanistic Modeling

- 1925-1960: Streeter-Phelps
  - DO modeling, based on BOD, SOD
- 1960-1970: Computerization
  - greater complexity, resolution possible
- 1970-1977: Biology
  - eutrophication modeling, based on N, P, light
- 1977-present: Toxics
  - partitioning of hydrophobics, complex physical, chemical and biological transformations

Evolving Issues

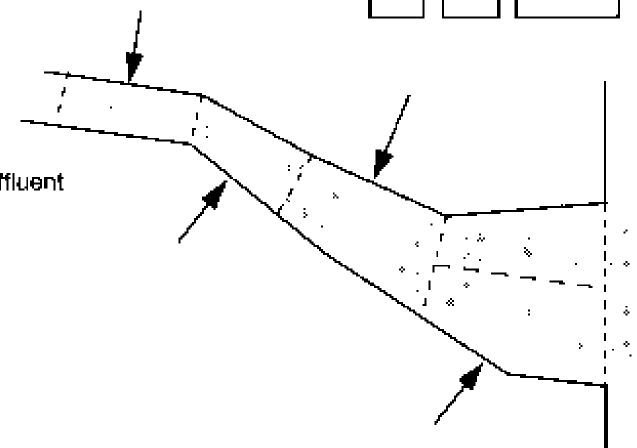
1925–1960 (Streeter-Phelps)

Problems: untreated and primary effluent
Pollutants: BOD/DO
Systems: streams/estuaries (1D)
Kinetics: linear, feed-forward
Solutions: analytical



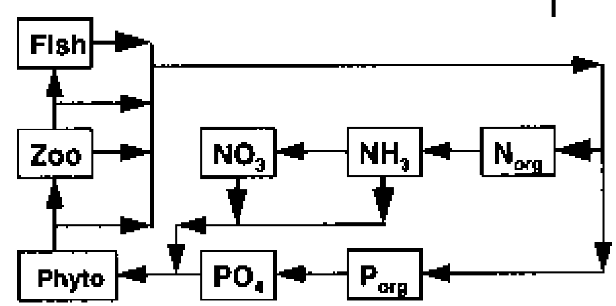
1960–1970 (computerization)

Problems: primary and secondary effluent
Pollutants: BOD/DO
Systems: estuaries/streams(1D/2D)
Kinetics: linear, feed-forward
Solutions: analytical and numerical



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

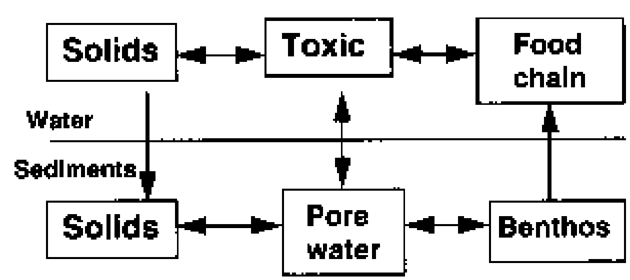


Figure 1.6 from Chapra, 1997

Economics of pollution control

- As standards become more strict
  - Costs go up disproportionally
  - Errors in judgment are more costly

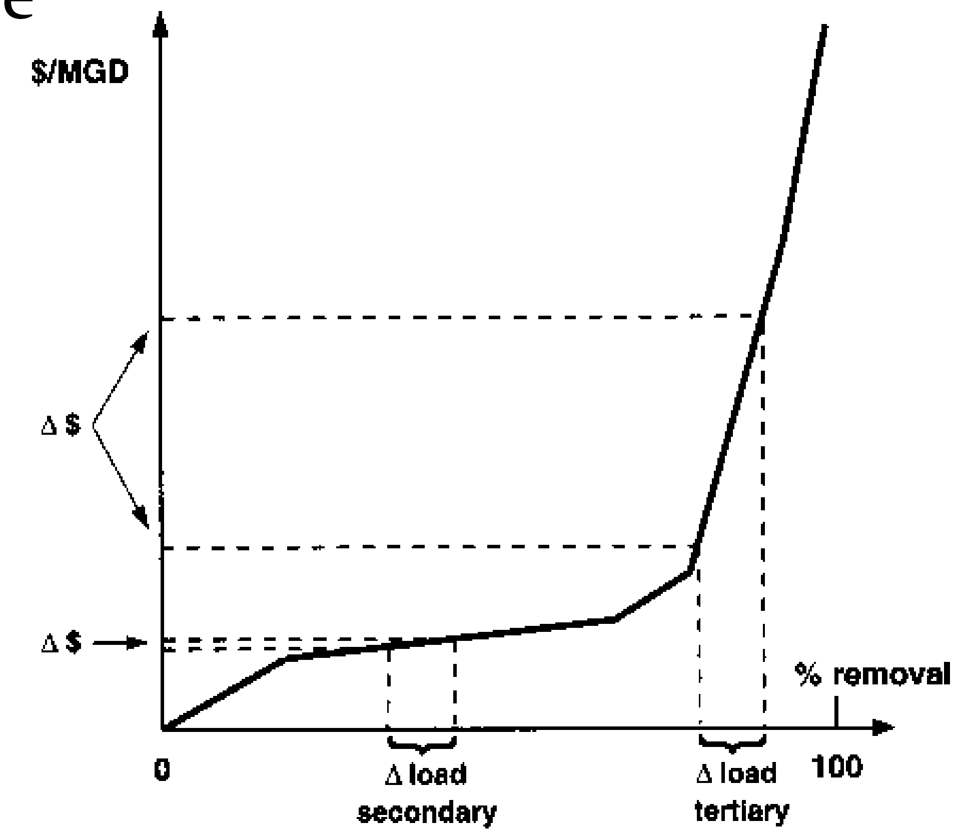


Figure 1.7 from Chapra, 1997

- To next lecture