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I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

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THIRD AUTUMN WORKSHOP ON MATHEMATICAL ECOLOGY

(14 October - 1 November 1996)

Outline of Lectures:
"I. Environmental Water Quality and Assessment
II. Fate and Effects of Toxicants in Aquatic Ecosystems"

Robert V. Thomann
Environmental Engineering Department
Manhattan College
New York, N.Y. 10471
U.S.A.

AUTUMN COURSE IN MATHEMATICAL ECOLOGY

ROBERT V. THOMANN

OUTLINE OF LECTURES

I. ENVIRONMENTAL WATER QUALITY AND ASSESSMENT

- INTRODUCTION
  - BASIC MANAGEMENT ISSUES
  - NEED FOR PREDICTIVE FRAMEWORKS
- GENERAL STRUCTURE OF WATER QUALITY MODELS
- WATER QUALITY PROBLEM APPLICATIONS
  - WATER BORNE DISEASE ORGANISMS
  - CHEMICALS
  - DISSOLVED OXYGEN
  - NUTRIENTS
- EXAMPLE CASE STUDIES

II. FATE AND EFFECTS OF TOXICANTS IN AQUATIC ECOSYSTEMS

- INTRODUCTION: UNIQUENESS OF TOXICS IN AQUATIC ECOSYSTEMS
- MODELS FOR PHYSICO-CHEMICAL TRANSPORT AND KINETICS
- MODELS FOR BIOACCUMULATION
- APPLICATION TO:
  - ORGANIC CHEMICALS (PCBs, PAHs)
  - METALS
- EXAMPLE CASE STUDIES

THREE PRINCIPAL MANAGEMENT REQUIREMENTS

- **QUANTITATIVE DIAGNOSIS OF WHO IS REPONSIBLE FOR PERCEIVED "PROBLEM"**
  - REGULATOR: RANKING OF INPUT CONTRIBUTIONS
  - REGULATED: "HOW MUCH AM I CONTRIBUTING TO THE PROBLEM?"
- **QUANTITATIVE PREDICTIONS**
  - RANGE OF FEASIBLE REDUCTIONS OF INPUT NUTRIENT LOADS
  - EXPECTED WATER QUALITY OUTCOMES OF NUTRIENT CONTROL PROGRAMS
- **UNDERSTANDING OF BEHAVIOR OF WATER BODY**
  - REDUCE "RESPONSE SURPRISES"

FOUR "FEARS OF ENVIRONMENTAL MANAGERS

- REDUCING INPUTS TO THE ENVIRONMENT WITH LITTLE OR NO SUBSEQUENT IMPROVEMENT IN ENVIRONMENTAL QUALITY

- CONTINUED ENFORCEMENT OF COSTLY CONTROL POLICIES WITH NO CHANGE IN ENVIRONMENTAL BENEFITS

- UNFORESEEN NEGATIVE ENVIRONMENTAL RESPONSE FROM A CONTROL PROGRAM SEEN AS BENEFICIAL

- LITIGATION

RATIONALE FOR MODELS

- **QUESTIONS ARE MORE COMPLEX**
  - NOT SUFFICIENT TO REDUCE NUTRIENT LOAD AND "SEE WHAT HAPPENS"
- **ECONOMIC AND POLICY IMPLICATIONS OF DECISIONS ARE MORE SIGNIFICANT AND WIDESPREAD**
  - e.g., WATERSHED & AIRSHED NUTRIENT INPUTS
- **ENFORCEMENT OF REGULATIONS ALWAYS SUBJECT TO VARYING INTERPRETATIONS & POSITIONS**
  - SCIENTIFIC CREDIBILITY INCREASINGLY MORE ESSENTIAL

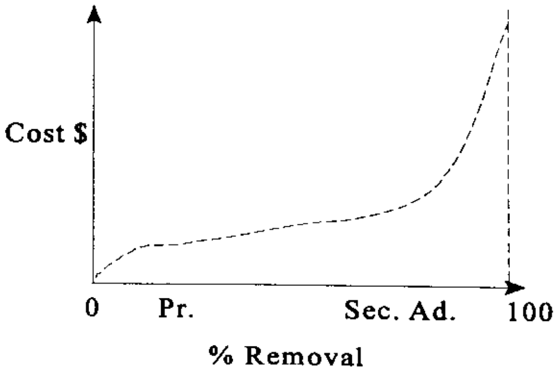
LEVELS OF TREATMENT
OF
MUNICIPAL AND INDUSTRIAL
WASTE

1. Screens, Removal of Solids (Floatables)
    "Preliminary"

2. Primary Treatment
    Solids Removal - Settling
    Organic Matter Removal - 30%

3. Secondary Treatment
    Primary & Biological Treatment

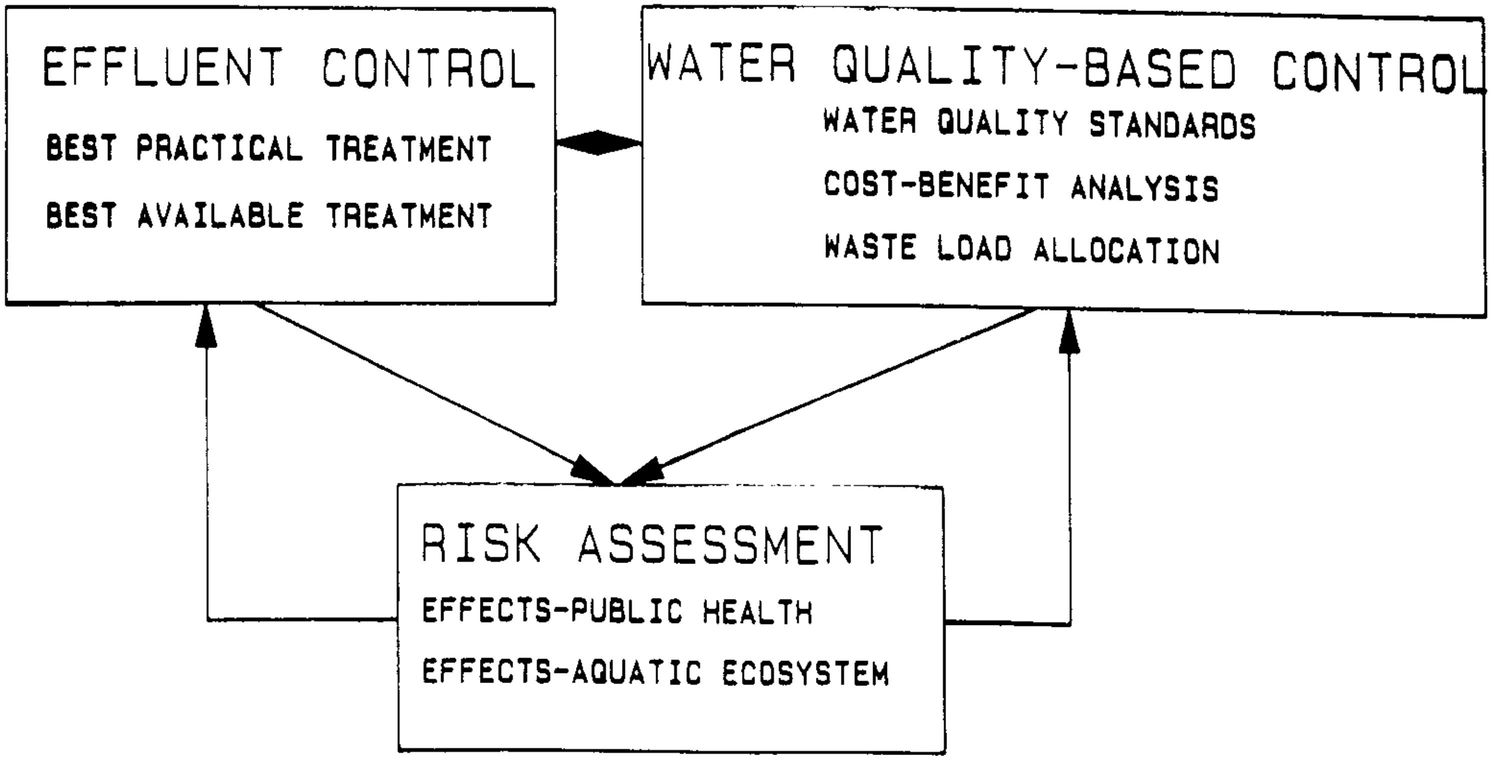
4. Advanced Treatment
    Nutrient Removal
    Additional Organic Matter Removal



FOUR "FEARS" OF ENVIRONMENTAL MODELERS

- BUILDING MODELS THAT PROVIDE LITTLE INSIGHT OR PREDICTIVE POWER
- DISCOVERING A "FATAL FLAW" IN A MODEL THAT IS BEING WIDELY USED
- CONTINUING TO DEVELOP MODELS THAT NO ONE IS USING
- BUILDING A MODEL THAT COLLAPSES OF IT'S OWN WEIGHT OF COMPLEXITY

PRINCIPAL ALTERNATIVE CONTROL OPTIONS



EFFLUENT CONTROL

BEST PRACTICAL TREATMENT

BEST AVAILABLE TREATMENT

WATER QUALITY-BASED CONTROL

WATER QUALITY STANDARDS

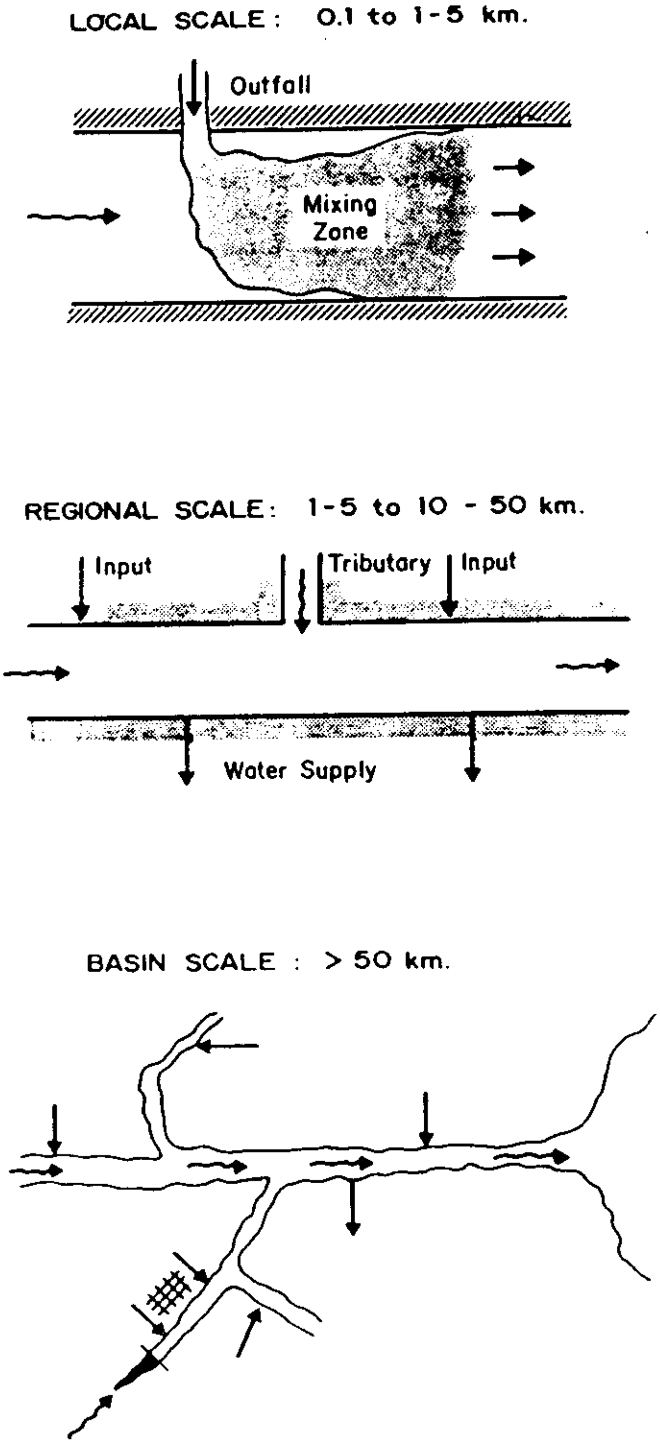
COST-BENEFIT ANALYSIS

WASTE LOAD ALLOCATION

RISK ASSESSMENT

EFFECTS-PUBLIC HEALTH

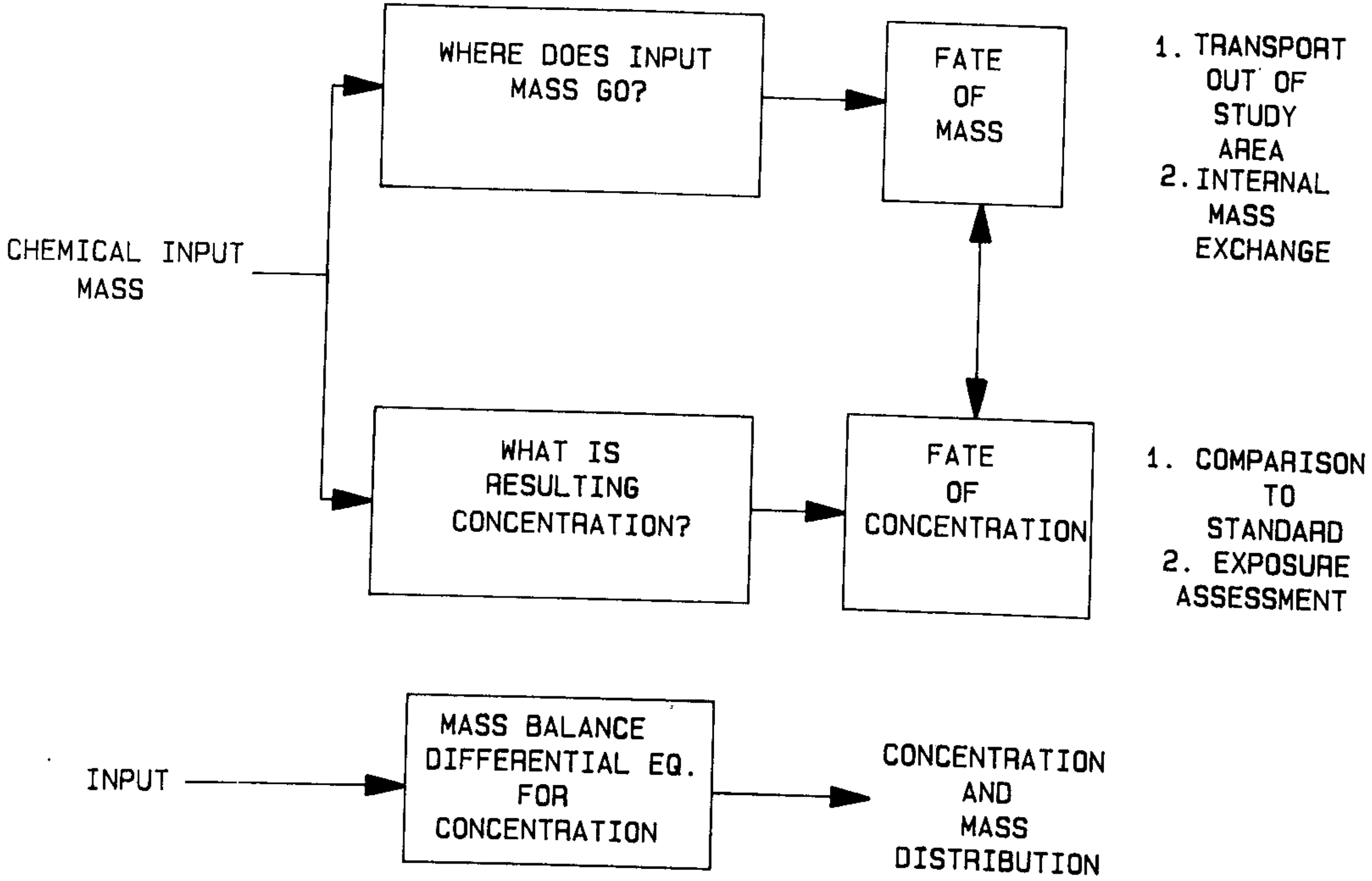
EFFECTS-AQUATIC ECOSYSTEM


LOCAL SCALE: 0.1 to 1-5 km.

REGIONAL SCALE: 1-5 to 10 - 50 km.

BASIN SCALE : > 50 km.

Fig. 3-1: SPACE SCALES FROM LOCAL TO BASIN WIDE THAT MAY HAVE TO BE CONSIDERED IN TOXIC SUBSTANCES EVALUATIONS


CHEMICAL INPUT MASS
WHERE DOES INPUT MASS GO?
FATE OF MASS
1. TRANSPORT OUT OF STUDY AREA
2. INTERNAL MASS EXCHANGE
WHAT IS RESULTING CONCENTRATION?
FATE OF CONCENTRATION
1. COMPARISON TO STANDARD
2. EXPOSURE ASSESSMENT
INPUT
MASS BALANCE DIFFERENTIAL EQ. FOR CONCENTRATION
CONCENTRATION AND MASS DISTRIBUTION

FUNDAMENTAL PRINCIPLE OF ALL WATER QUALITY MODELS
MASS BALANCE

DIFFERENTIAL EQUATION FORM:
(FOR CONTROL VOLUME, V_i)

$$V_i \, dc_i / dt = \text{INPUT} +/- \text{TRANSPORT \& DISPERSION}$$

+/- ATMOS. EXCHANGE
+/- SEDIMENT EXCHANGE
- DECAY PROCESSES

SOLUTION:

CONCENTRATION @ LOCATION i, AND TIME, $t = c(i, t)$

MASS BALANCE OVER A REGION:
AT TIME t

$$\sum_{i}^{R} V_i \, c(i, t)$$

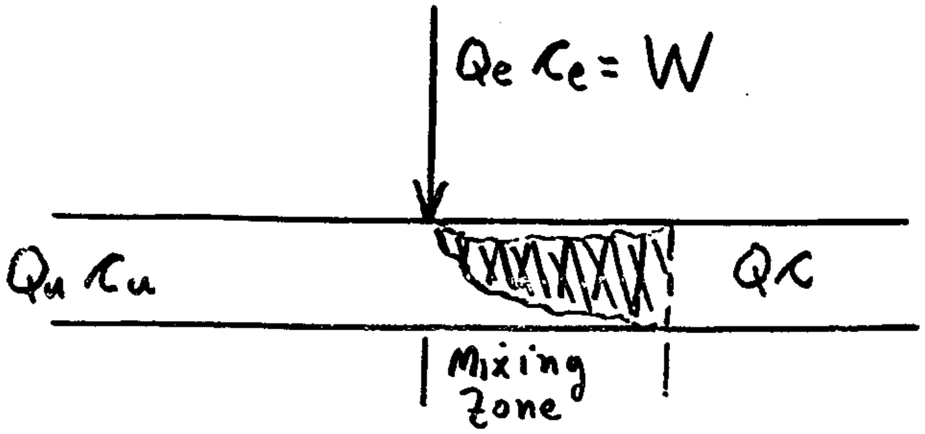
CUMULATIVE MASS BALANCE OVER TIME:

$$\sum_{0}^{T} \sum_{i}^{R} V_i \, c(i, t) = \sum_{0}^{T} \sum_{i}^{R} \{\text{INPUT} +/- \text{TRANSPORT}\ldots.\} = \sum_{i}^{R} M(t)$$

ANNUAL MASS FLUX:

$$[\sum_{i}^{R} M(t + 1 \text{ YEAR}) - \sum_{i}^{R} M(t)] / 1 \text{ YEAR}$$

Principle: For single source,
maximum concentration in
river occurs at outfall.



Concentration after complete mixing:

$$c = \frac{Q_u c_u + Q_e c_e}{Q}$$
$$= c_u(1-\phi) + c_e\phi$$

where:

$$\phi = \frac{Q_e}{Q} = \frac{Effluent\ Flow}{Total\ River\ Flow}$$

For $c_u = 0$: $$c = \frac{W}{Q}$$

Then allowable discharge:

$$\underline{(W)_{\text{allow}} \leq c_r\, Q - c_u Q_u}$$

where c_r = water quality standard
$\Rightarrow$ Risk Level

Allowable effluent concentration:
$(c_u = 0)$

$$\underline{(c_e)_{\text{allow}} \leq c_r/\phi}$$

Questions:

1) What c_r should be used?
2) What river flow should be used?

Fig. 3-2: DISTANCE TO 95% REDUCTION OF MAXIMUM CONCENTRATION AT OUTFALL (NO DILUTION AND NO TRIBUTARY INFLOWS)

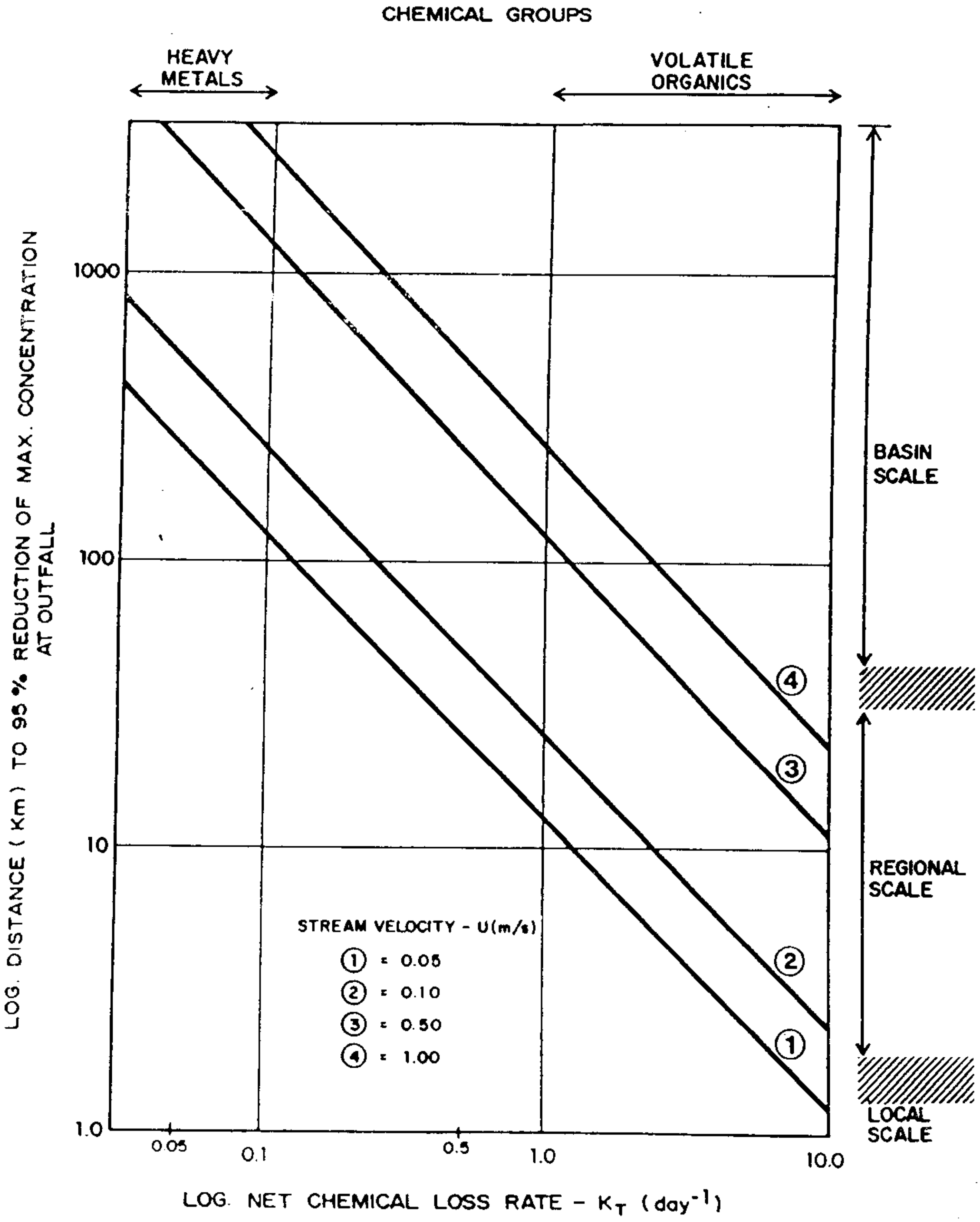


Fig. 3-4: MASS BALANCE AT OUTFALL

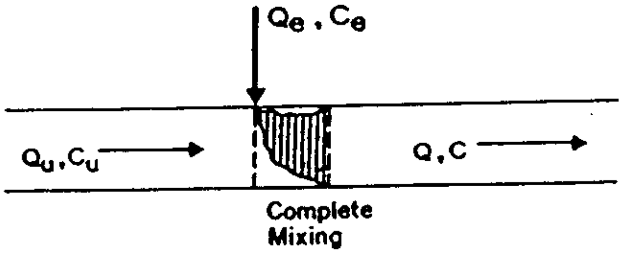


Fig. 3-5: EFFECT OF DILUTION ON IN-STREAM WATER QUALITY STANDARD AND RESULTING RELATIVE RISK. CARBON TETRACHLORIDE AS EXAMPLE, SEE TABLE 2-1 AND 2-2 FOR CRITERION.

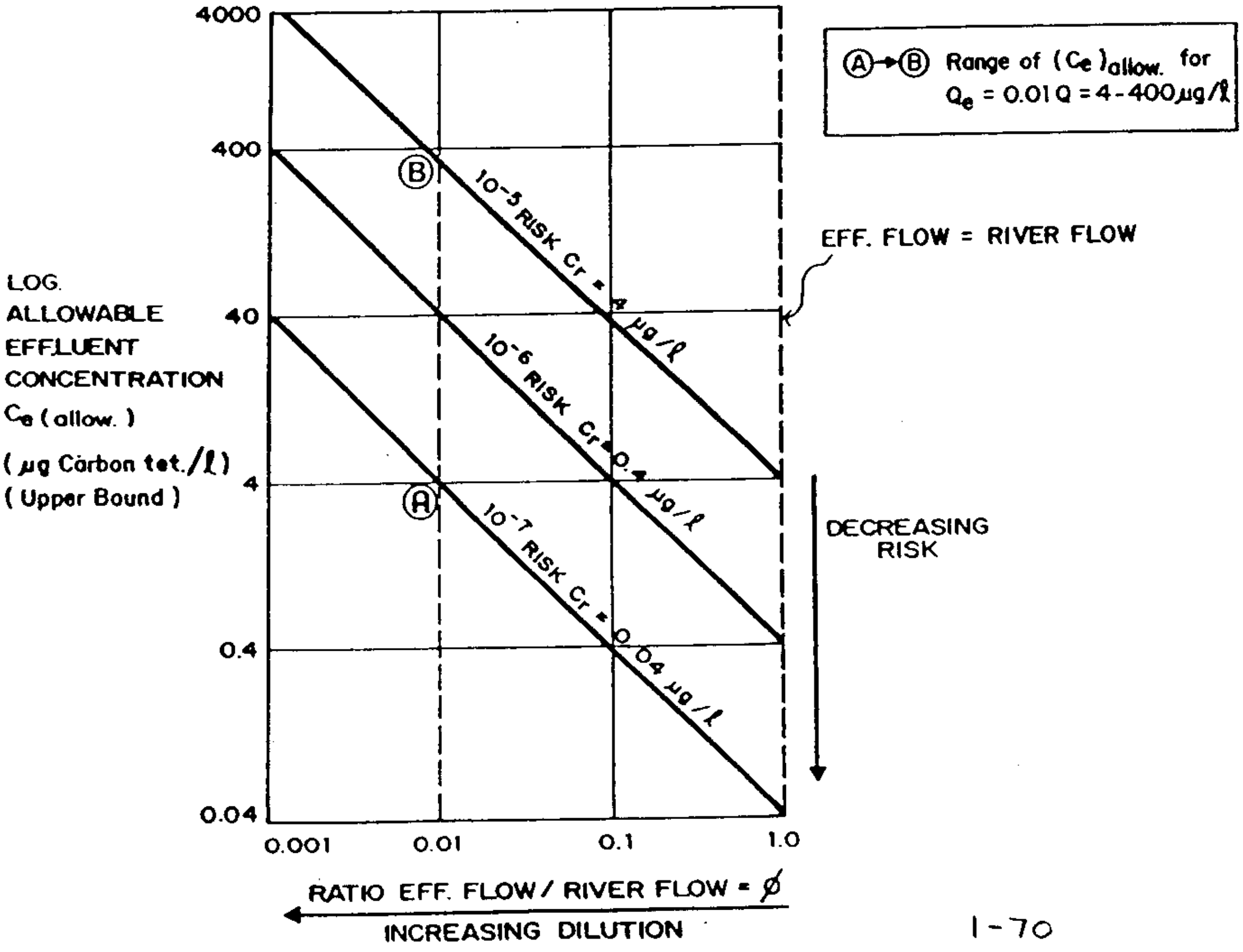


Fig. 3-7 : ILLUSTRATION OF POSSIBLE DOWNSTREAM FATE OF CHEMICALS OR TOXICITY

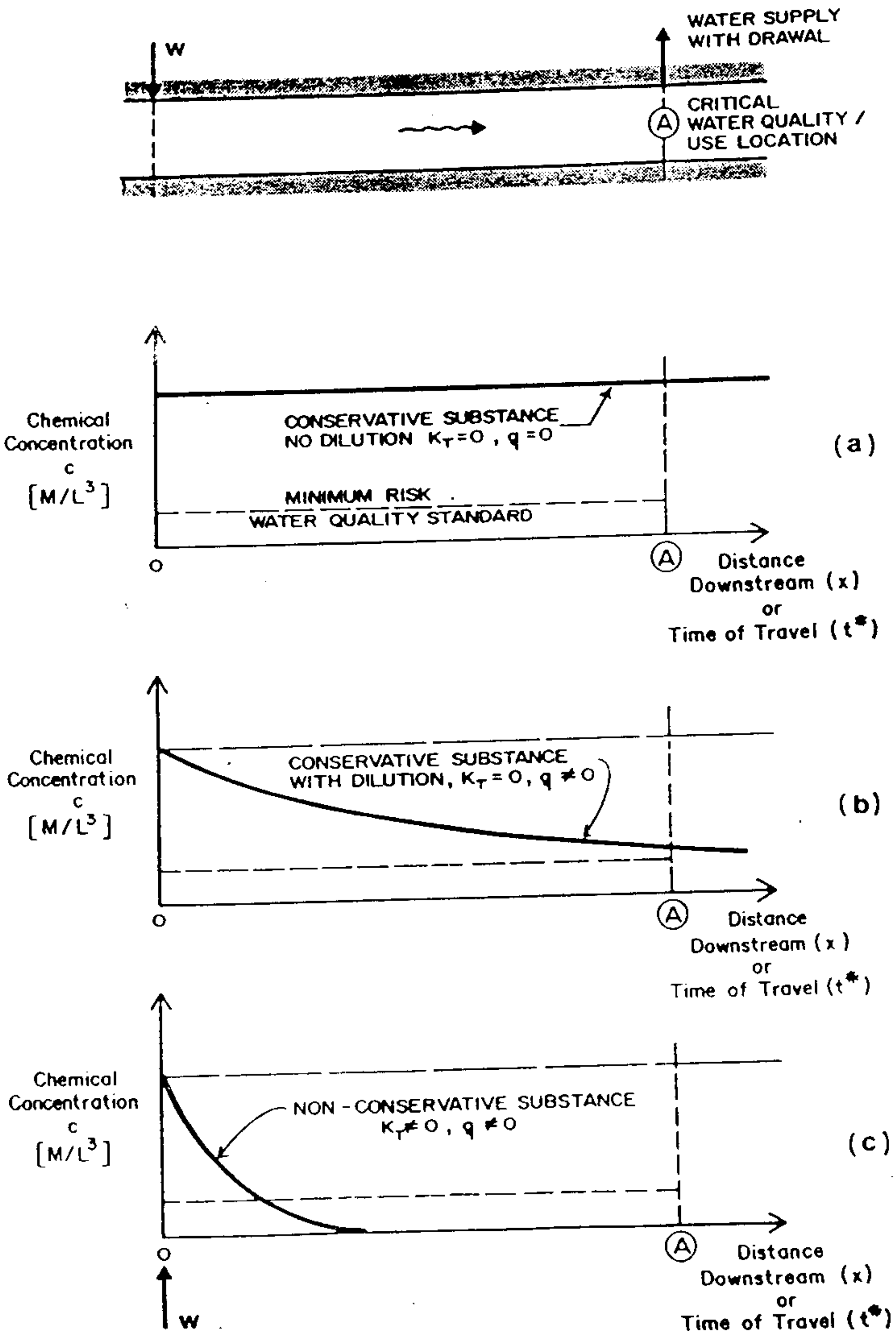
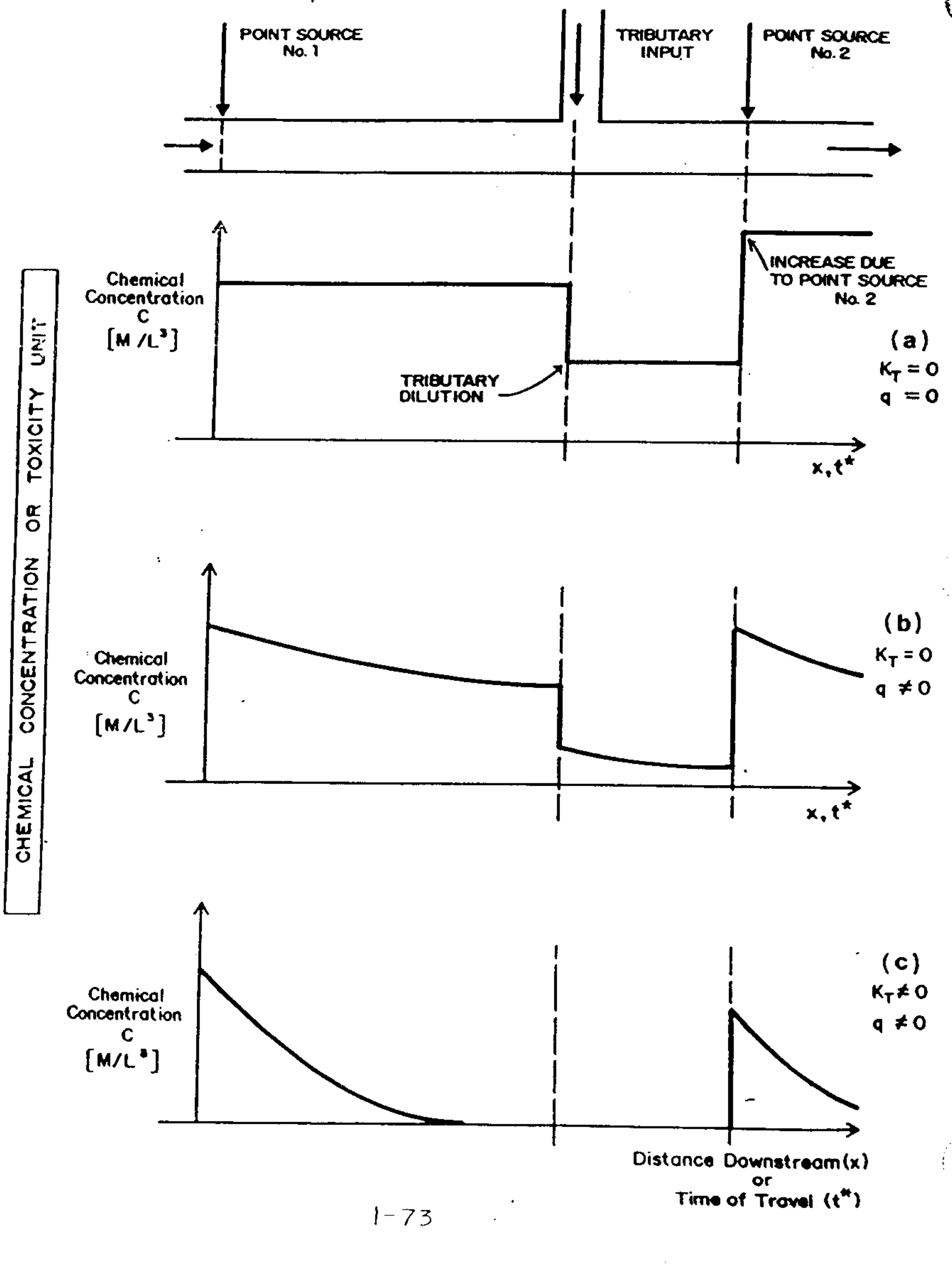


Fig. 3-8 : SCHEMATIC OF IMPACT OF INCREASING TURBIDITY ON ADDITIONAL DOWNSTREAM POINT SOURCE INPUT



THE WATER BORNE DISEASE ISSUE

I. Background

1. Problem: In Latin America: gastroenteritis and diarrheal diseases ≈ 200,000 deaths/yr or risk of almost 1/1000
   cholera: 500,000 ill, 5000 deaths

   Water Uses: Water Supply
   Shellfish & Fish
   Water Contact Recreation

2. Inputs:
   - Raw Sewage
   - Point Municipal, w/wo chlorination
   - Tributary Runoff

3. Water Quality Responses:
   - Steady State
   - Storm Related Transients

Indicator Bacteria, Pathogens & Viruses

Indicator Bacteria
Total Coliform
Fecal Coliform $K \approx 1\text{-}3/\text{day}$
Fecal Streptococci

Pathogens
Cholerae - cholera
Salmonellae - typhoid
Shigella - dysentery

Viruses
Enteroviruses - polio
$K \approx 0.1\text{-}0.3/\text{day}$
Reoviruses
•
• - Hepatitis
•

Pathogenic Protozoan
Giardia lambia
Entamoeba Hystolytica

III. KINETIC COMPONENTS FOR BACTERIA MODEL

1. Mortality & Losses
    - Sunlight
    - Temperature
    - Salinity
    - Settling
    - Predation
    - Chlorination
    - Toxics

   Gains
    - Aftergrowth
    - Sediment
    - Resuspension

2. Let K_B = net decay rate of bacteria (Mortality & Losses - Gains)

$$= K_{B1} + K_{BI} + K_{Bs}$$

where

K_{B1} = base death rate = f (T, sal.)
K_{BI} = death rate due to sunlight
K_{Bs} = net loss (gain) due to settling (resuspension) and/or after growth

3. Order of K_B for Total/Fecal Coliform Bacteria:

0.5-3.5/day Freshwater, 20°C
2-7/day Sea water, 20°C

T_{90} (Time to 90% mortality):
0.7-4.6 Days Freshwater
0.3-1.0 Days Sea water

4. Effect of Sunlight:

English Studies (Gameson & Gould, 1974)

% Freq of Occurrence of Decay Rate (≥)	K_B (1/day)	T_{90} (hours)
5	80	0.7
50	18	3.1
95	9	6.1

5. Two Model Levels

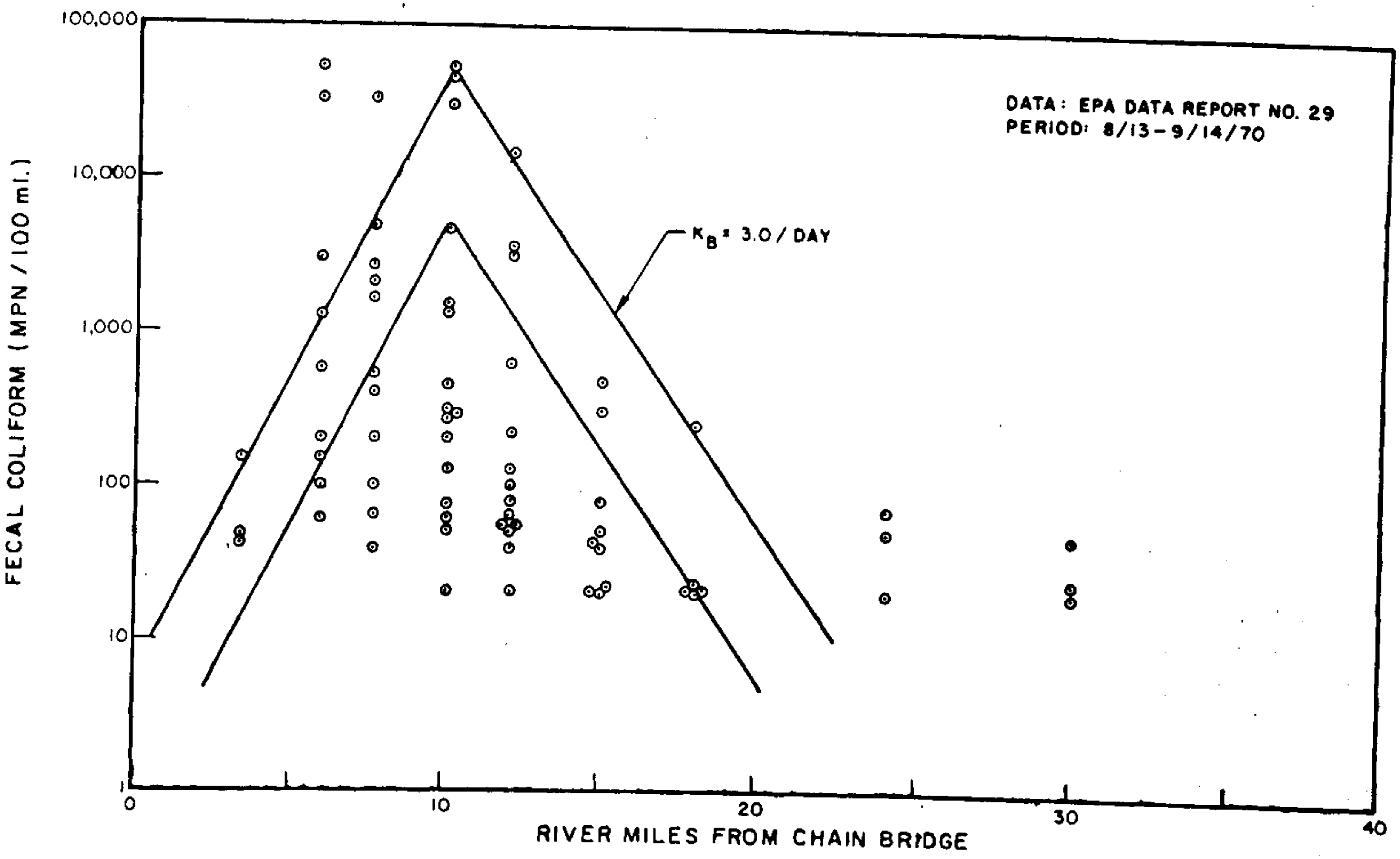
A. Simple First Order Loss Rate
(function of temperature)

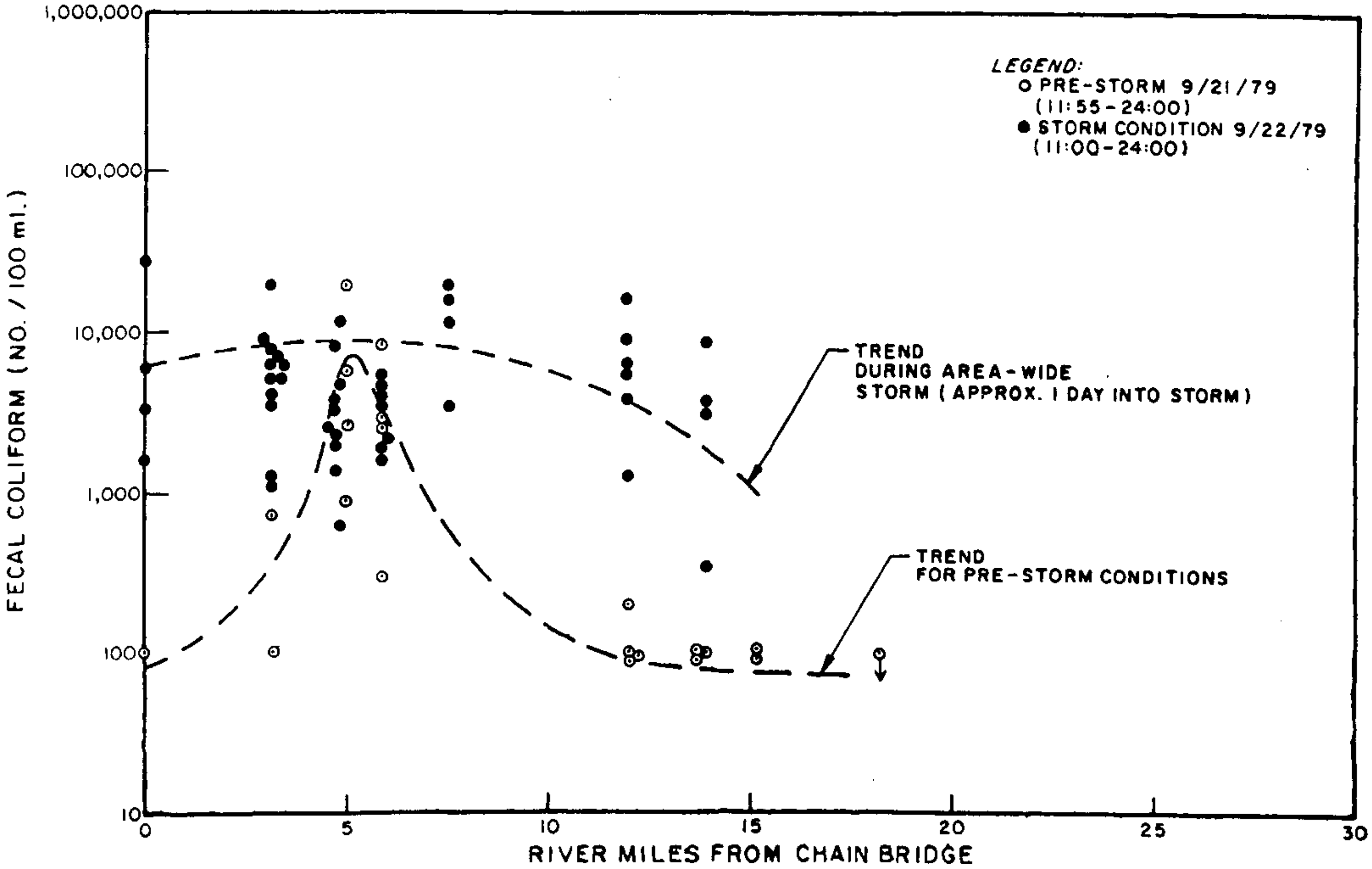
$$\frac{dc_B}{dt} = \text{Inputs} + \text{Transport} - K_B(T)\,c_B$$

B. $K_B = f(T, \text{sal.}, I, \upsilon_s)$ averaged over depth

where

$$K_B = [[0.8 + 0.006(\%\ \mathit{seawater})] \bullet 1.07^{T-20}] + \frac{I_o(t)}{K_e H}(1 - e^{-K_e H}) + \nu_s / H$$


DATA: EPA DATA REPORT NO. 29
PERIOD: 8/13-9/14/70
K_B = 3.0/DAY
FECAL COLIFORM (MPN / 100 ml.)
100,000
10,000
1,000
100
10
1
0
10
20
30
40
RIVER MILES FROM CHAIN BRIDGE



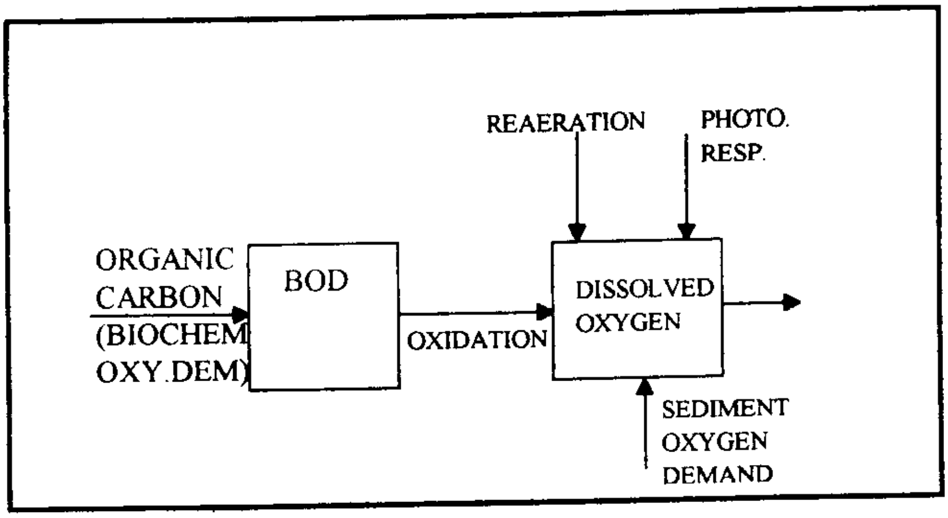
FIGURE

TRENDS IN FECAL COLIFORM CONCENTRATIONS PRIOR TO AND DURING STORM OF 9/22-25/79

(DATA FROM O'BRIAN & GERE ENG. INC. & LIMNO-TECH. INC.)

THE DISSOLVED OXYGEN PROBLEM

BASIC COMPONENTS:



MASS BALANCE FOR DISSOLVED OXYGEN CONCENTRATION (c) OVER A CONTROL VOLUME (V):

V dc/dt = - OXIDATION OF BOD CARBON & NITROGEN

- SEDIMENT OXYGEN DEMAND

+ REAERATION

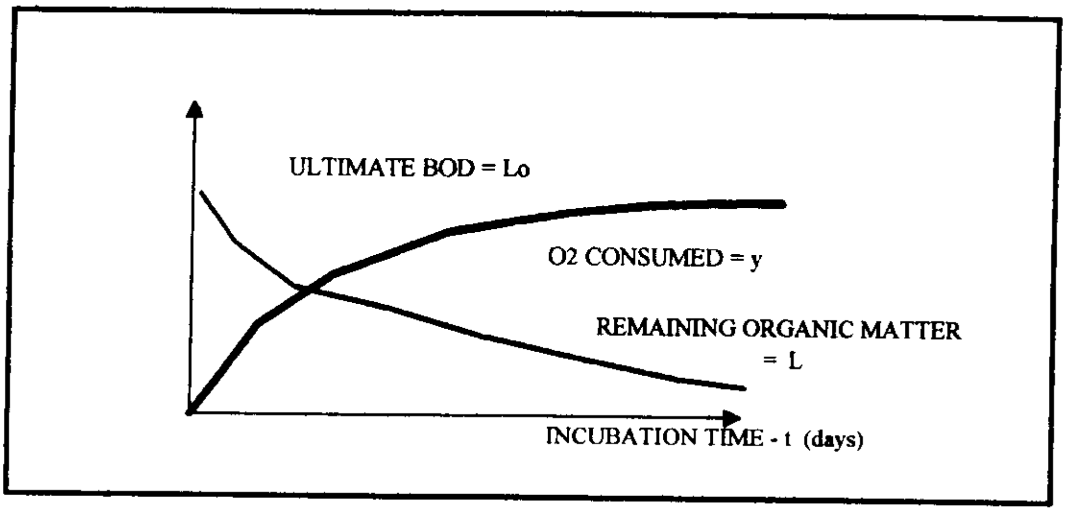
+ PHOTSYNTHESIS - RESPIRATION

+/- TRANSPORT & DISPERSION

BIOCHEMICAL OXYGEN DEMAND

THE OXYGEN EQUIVALENT OF THE ORGANIC CARBON CAPABLE OF UTILIZING OXYGEN FOR OXIDATION OF ORGANIC CARBON TO CO_2

MEASUREMENT: UPTAKE OF DO BY WATER SAMPLE IN BOD BOTTLE



BOD BOTTLE EQUATION:

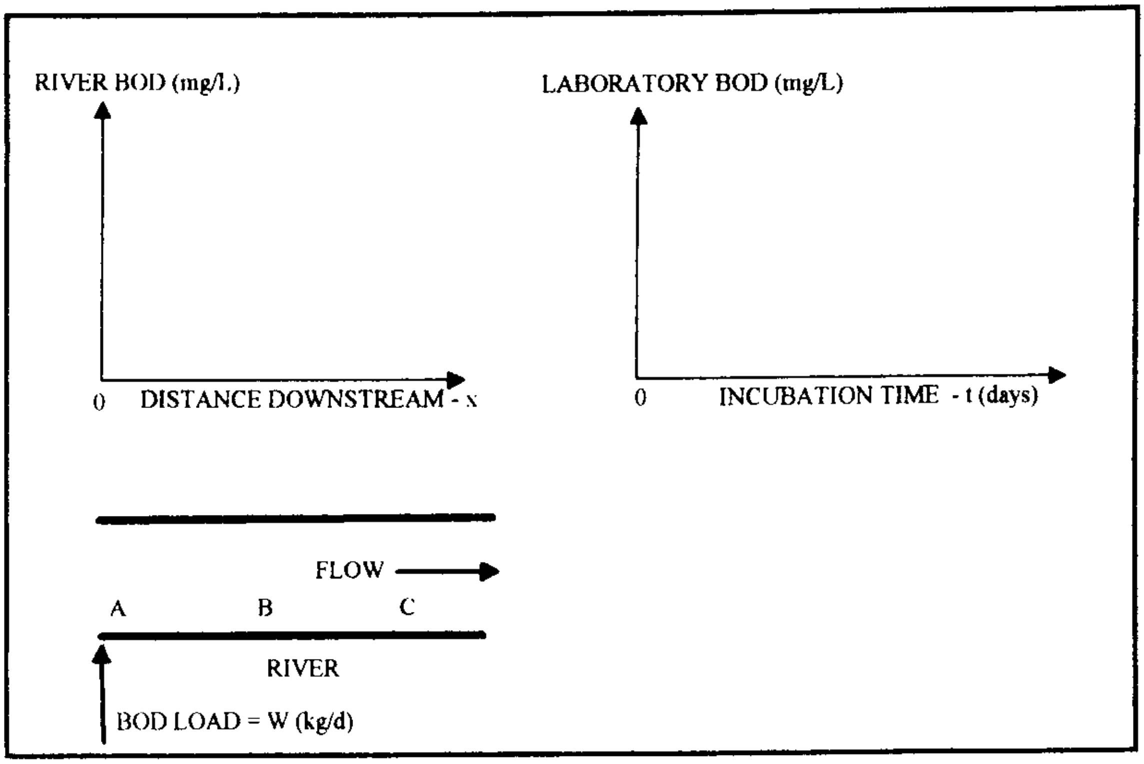
$dL/dt = -K_1L$; SOL'N: $L = L_o \exp(-K_1t)$

$y = L_o - L$

THEREFORE: $y = L_o(1 - \exp(-K_1t))$

USUALLY MESURE y_5 = 5 - day BOD

BOD OXIDATION IN RIVERS & STREAMS



U = RIVER VELOCITY (km/d)
K_r = RIVER BOD LOSS RATE (1/day)

$$U\, dL/dx = -K_r L$$

$$L = (L_O)_A \exp(-K_r x/U)$$

WHERE

$$(L_O)_A = [(L_O Q)_{up} + (L_O Q)_{eff}]/(Q_{up} + Q_{eff})$$

SIMPLIFIED DISSOLVED OXYGEN MODEL FOR RIVERS

@ STEADY STATE:

$$U\ dc/dx = K_a\,(c_s - c) - K_d\,L(x) + P - r - SOD$$

CONSIDERING ONLY BOD (= L(x))

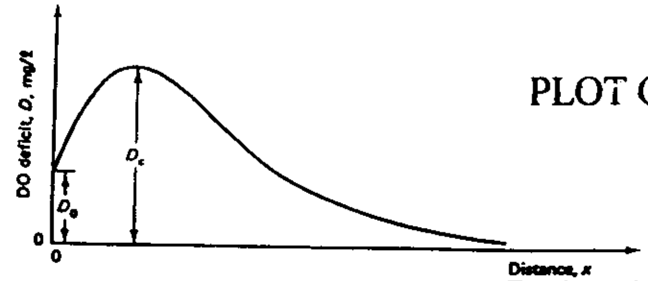
$$U\ dc/dx = K_a\,(c_s - c) - K_d\,L_O\,\exp(-K_r x/U)$$

DEINE D = DO DEFICIT = $c_s - c$

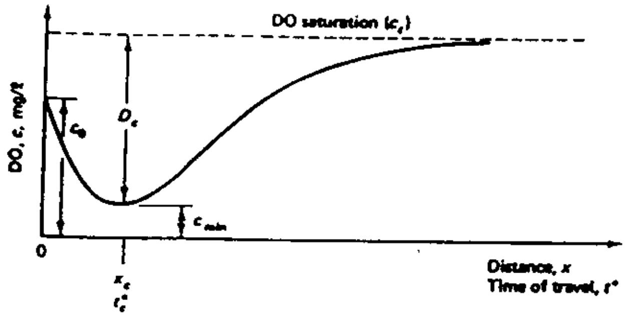
THEN SOLUTION IS:

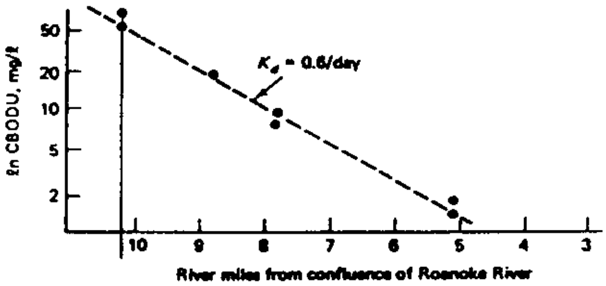
$$D = \frac{K_d (L_O)_A}{K_a - K_r}\left\{e^{-K_r x/U} - e^{-K_a x/U}\right\} + D_0 e^{-K_a x/U}$$

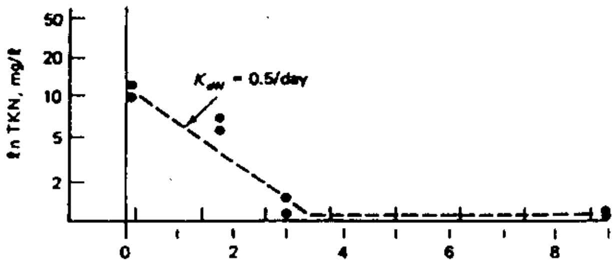
PLOT OF DO PROFILE
& EXAMPLE

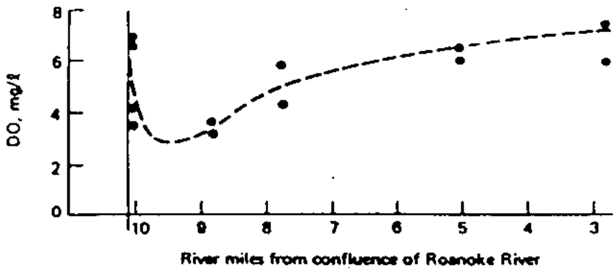


(a)

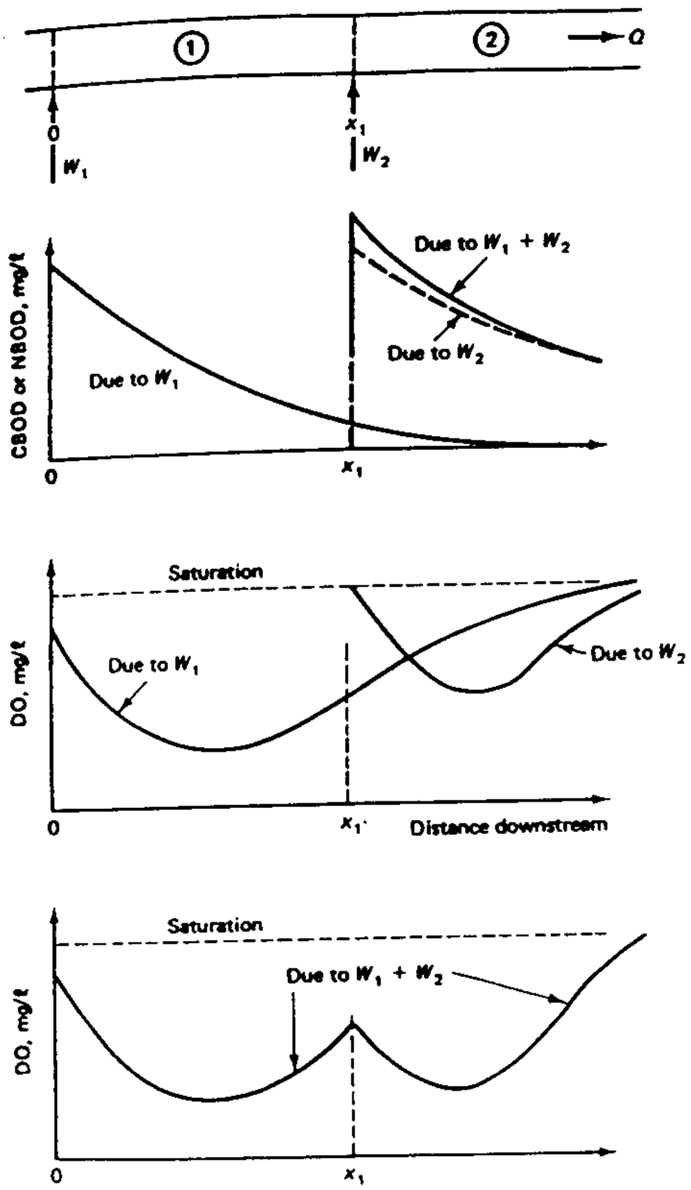








MULTIPLE INPUT CASE



INTERPRETATION OF N/p RATIO

BASIC PRINCIPLE:

PLANT BIOMASS CONTROLLED BY NUTRIENT AT LOWEST CONCENTRATION

AVAILABLE NUTRIENT (i.e. DIN, DIP) → PLANT BIOMASS (e.g., PHYTO. CHLOR.)

NUTRIENT UPTAKE & CONVERSION TO PLANT BIOMASS

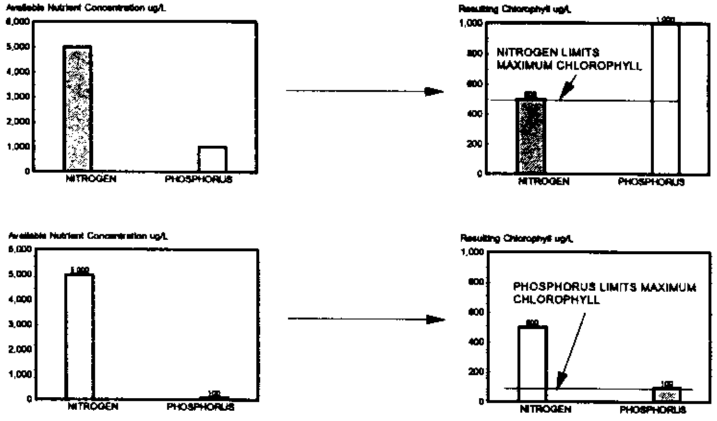
LET:

N = available nitrogen (DIN)
p = available phosphorus (DIP)
a_N = nitrogen/chlorophyll ratio
a_p = phosphorus/chlorophyll ratio
P = phytoplankton chlorophyll

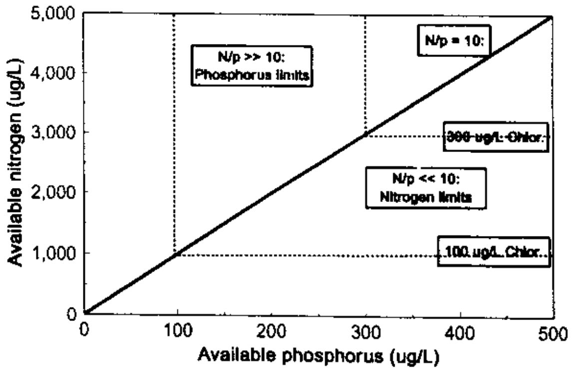
THEN, THE MAXIMUM BIOMASS IS GIVEN BY

$$P = \min\{ N/a_N;\ p/a_p \}$$

ASSUME: (1) NUTRIENT IN SHORTEST SUPPLY LIMITS MAXIMUM BIOMASS
(2) COMPLETE CONVERSION OF NUTRIENT TO BIOMASS
(3) NIT/CHLOR = 10 & PHOS/CHLOR = 1



NITROGEN & PHOSPHORUS LIMITATION



(From Thomann and Mueller, 1987)

ALGAL CELL STOICHIOMETRY

GLOBAL MEAN: "REDFIELD RATIOS" (Redfield et al, 1966)

ALGAL BIOMASS COMPOSITION: $C_{106}H_{263}O_{110}N_{16}P$

$$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4)$$

STOICHIOMETRY USING "REDFIELD" RATIOS					
C/N		C/p		N/p	
mole Basis	Weight Basis	mole Basis	Weight Basis	mole Basis	Weight Basis
6.63	5.68	106	41	16	7.22
C: 12 g/mole; N: 14 g/mole; P: 31g/mole					

BUT NOTE THAT AGAL STOICHIOMETRY VARIES AS FUNCTION OF AVAILABLE NUTRIENT:

e.g. CHESAPEAKE BAY (Cerco and Cole, 1994): C/N: 4.5 - 6 C/p: 30 - 75 N/p: 5 - 15

CARBON/CHLOROPHYLL: 30 - 140

For C/CHLOR = 50; C/N = 5 & C/p = 50

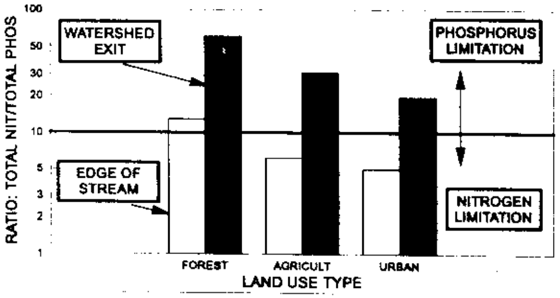
THEN N/p = 10; AND N/CHLOR = 10 & p/CHLOR = 1

SOME TN/Tp RATIOS FOR INPUT NUTRIENT LOADS AND MARINE WATERS

- POINT SOURCES:
  - w/o phos. removal = 3
  - with phos. removal = 30
- NONPOINT SOURCES:
  - Fertilizer & manure: 3
  - @edge of stream = 6
  - @watershed exit = 30
- MARINE WATERS (DIN/DIP) = 2

(Adapted from Thomann and Mueller, 1987 and Puckett, 1995)

CHANGE IN TN/TP FROM EDGE OF STREAM TO WATERSHED EXIT



Compiled from Aqua Terra (1992) & Thomann & Mueller, (1987)

LIMITING NUTRIENTS FOR VARIOUS WATER BODIES

- RIVERS & STREAMS:
  - PS dominated
    - w/o phos. removal: N/p <<10; N limited
    - with phos. rem.: N/p >>10; p limited
  - NPS dominated: N/p >> 10; p limited
- ESTUARIES:
  - Fresh Water region
    - PS dominated: N/p << 10; N limited
    - NPS dominated: N/p >> 10; p limited
  - Saline region: N/p << 10; N limited
  - Transition region, Brackish: N or p limited
- LAKES:
  - NPS dominated: N/p >> 10; p limited
  - PS dominated: N/p << 10; N limited

(From Thomann and Mueller, 1987)

SIMPLE LAKE ANALYSIS:
VOLLENWEIDER MODEL

- ASSUMPTIONS:
  - COMPLETELY MIXED LAKE
  - STEADY STATE
  - PHOSPHORUS LIMITATION
  - TOTAL PHOS. = MEASURE OF TROPHIC STATE
- BASIC EQUATION:

$$V\,dp/dt = \underbrace{W}_{\boxed{\text{INPUT MASS}}} - \underbrace{vAp}_{\boxed{\text{NET MASS LOSS FROM WATER COLUMN}}} - \underbrace{Qp}_{\boxed{\text{MASS OUTFLOW}}} = 0$$

NORMALIZING BY WATER SURFACE AREA:

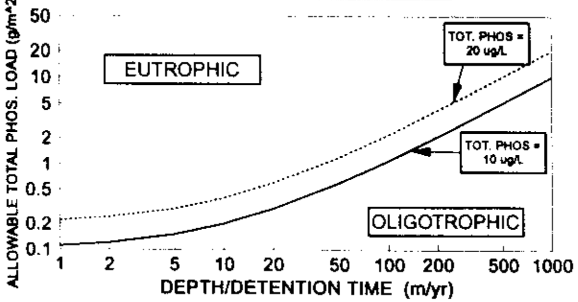
$p = (W'\backslash A)/(q + v)$

where q = Q/A = hydraulic overflow rate (m/yr)
= depth/detention time
v = net effective loss velocity of total phosphorus(m/yr)

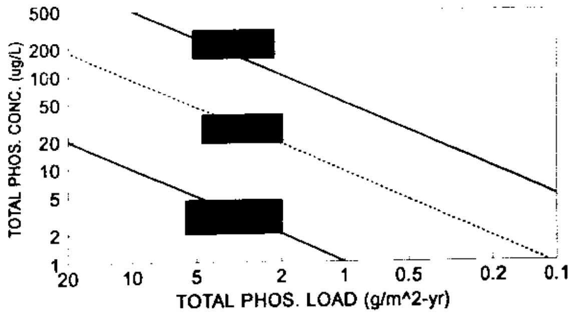
From data on North temperate Lakes:
VOLLENWEIDER: v = 10 m/yr (approx. aver.)

Allow. TP Areal Load (g/m^2-yr) = (0.01)*(10 + H/det t)

THE VOLLENWEIDER PLOT



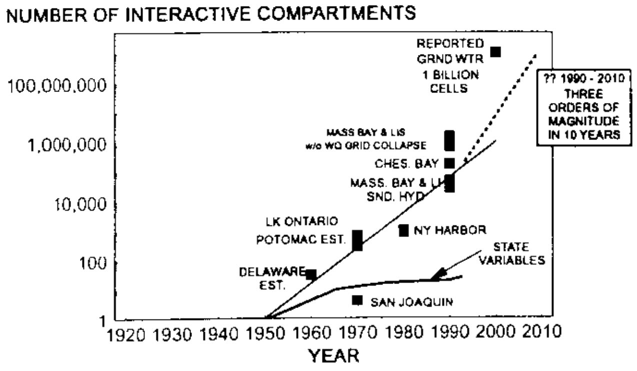
TOTAL PHOS. IS LINEAR TO INPUT LOAD



ISSUES

- TIME VARIABLE BEHAVIOR
  - VARIABLE HYDROLOGY & HYDRODYNAMICS
  - SPRING INPUT OF NPS LOADS
  - RESPONSE TIME FOR WATER BODY TO REACH WQ OBJECTIVE
- SPATIALLY VARIABLE BEHAVIOR (1 - 3 DIMENSIONS)
  - COVES, EMBAYMENTS, BAYS
  - ESTUARY/COASTAL OCEAN
- PLANT/NUTRIENT
  - NITROGEN/PHOS. LIMITATION
  - PLANT GROWTH/DEATH KINETICS
- SEDIMENT
  - NUTRIENT FLUXES
  - SEDIMENT OXYGEN DEMAND

INCREASE IN SIZE OF WATER QUALITY MODELS

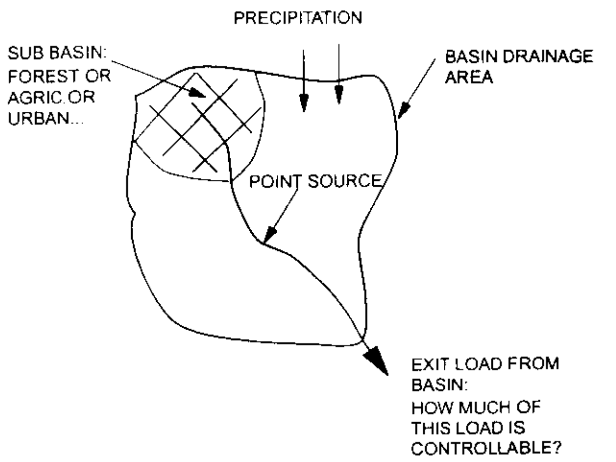


1950 - 1990 ORDER OF MAGNITUDE
INCREASE EVERY DECADE

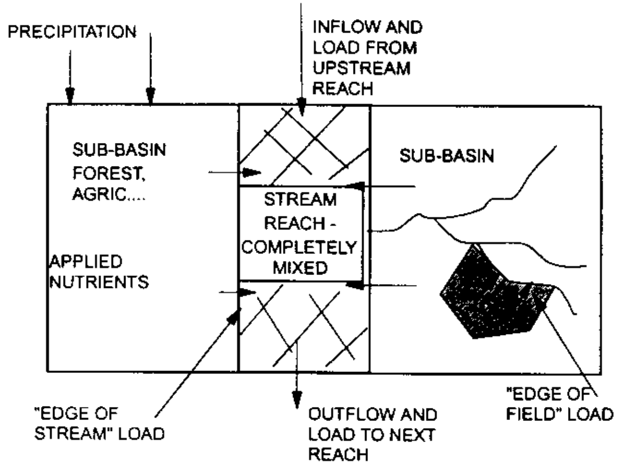
CHESAPEAKE BAY WATER QUALITY MODEL
22 STATE VARIABLES

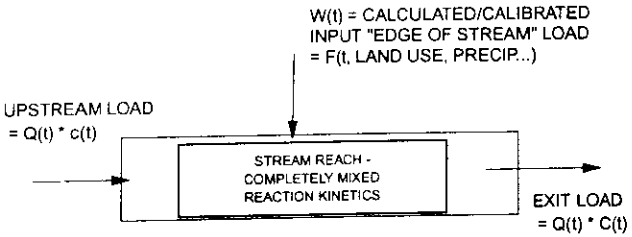
- PHYTOPLANKTON (3)
  - DIATOMS, CYANOBACTERIA, OTHERS
- CARBON (3)
  - DISSOLVED ORGANIC CARBON
  - LABILE PARTICULATE ORGANIC CARBON
  - REFRACTORY PARTICULATE ORGANIC C.
- NITROGEN (5)
  - AMMONIUM, NITRATE
  - DISSOLVED ORG. N, LABILE PART. ORG. N & REFRACTORY PART. ORG. N.
- PHOSPHORUS (5)
  - TOTAL PHOSPHATE, ACTIVE METAL
  - DISS. ORG. P, LABILE PART. ORG. P & REFRACTORY PART. ORG. P.
- SILICA: DISS. & PART. (2)
- DISSOLVED OXYGEN, CHEMICAL OXYGEN DEMAND (2)
- SALINITY & TEMPERATURE (2)

MOTIVATION FOR WATERSHED MODELING

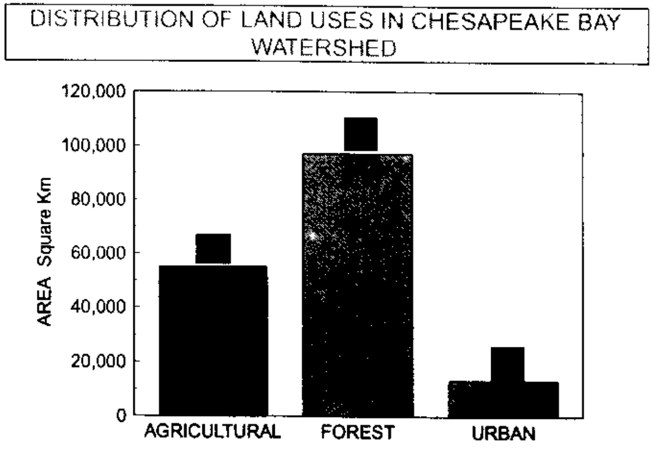


BASIC COMPONENTS OF WATERSHED MODEL

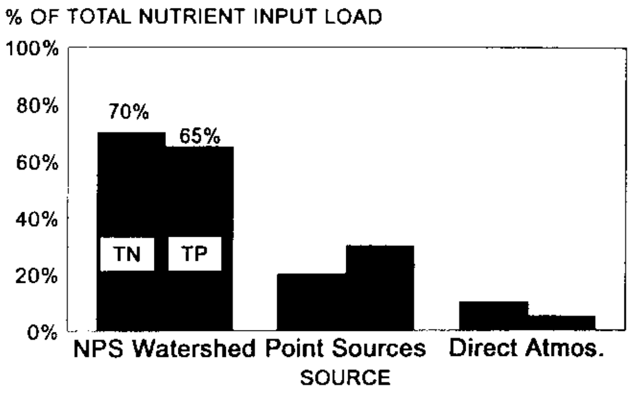




$$dc(t)V(t)/dt = (Q(t) * c(t))up + W(t) - (Q(t)*c(t))dwn - R(t)$$

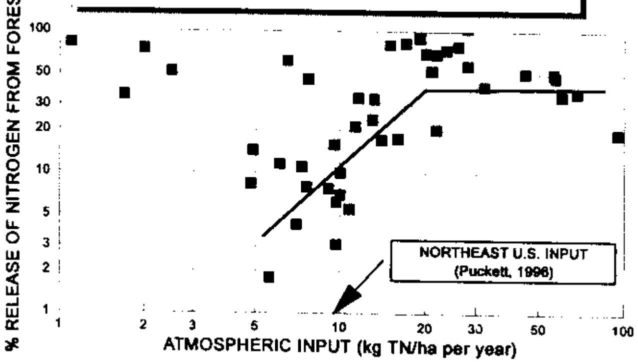

DISTRIBUTION OF LAND USES IN CHESAPEAKE BAY WATERSHED

CONTRIBUTION OF PRINCIPAL SOURCES TO TOTAL NITROGEN & LOAD

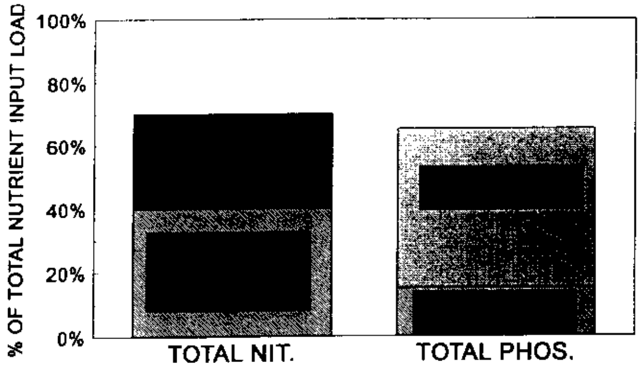


% RELEASE OF NITROGEN FROM FORESTS

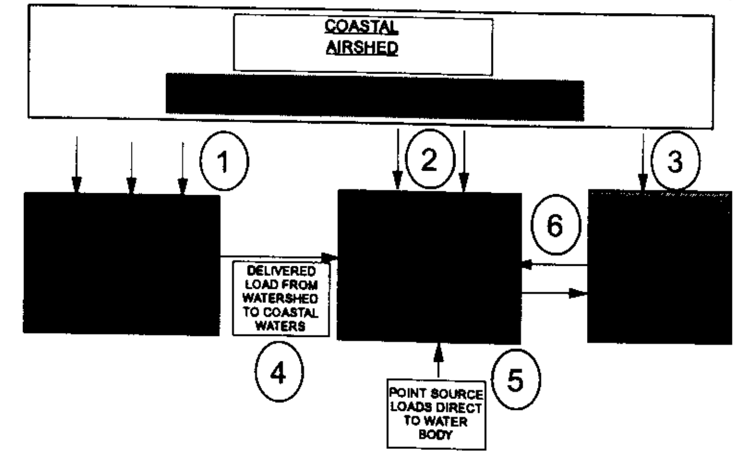
(Data from Hunsacker et al, 1994)



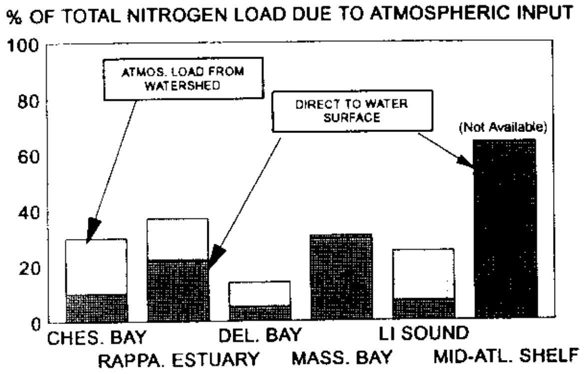
CONTROLLABILITY OF TOTAL NITROGEN & *NPS WATERSHED* LOADS



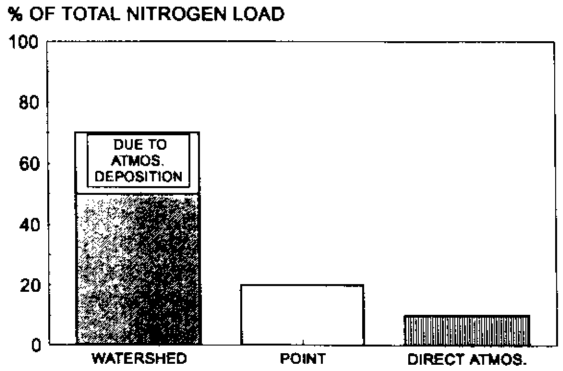
COMPONENTS OF NITROGEN LOADING TO COASTAL WATERS

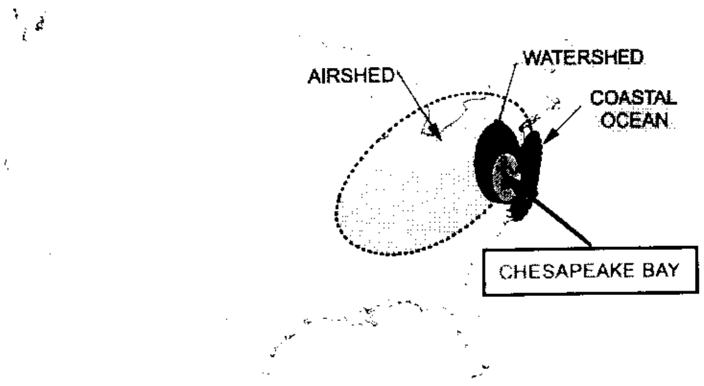


CONTRIBUTION OF ATMOS. NITROGEN DEPOSITION DELIVERED THROUGH WATERSHED



CONTRIBUTION OF ATMOSPHERIC DEPOSITION TO WATERSHED DELIVERED LOAD CHESAPEAKE BAY





THE INCREASING SCALE OF MODEL/MANAGEMENT DOMAIN

INCREASE IN AREA OF INTEREST FOR WATER QUALITY OF CHESAPEAKE BAY