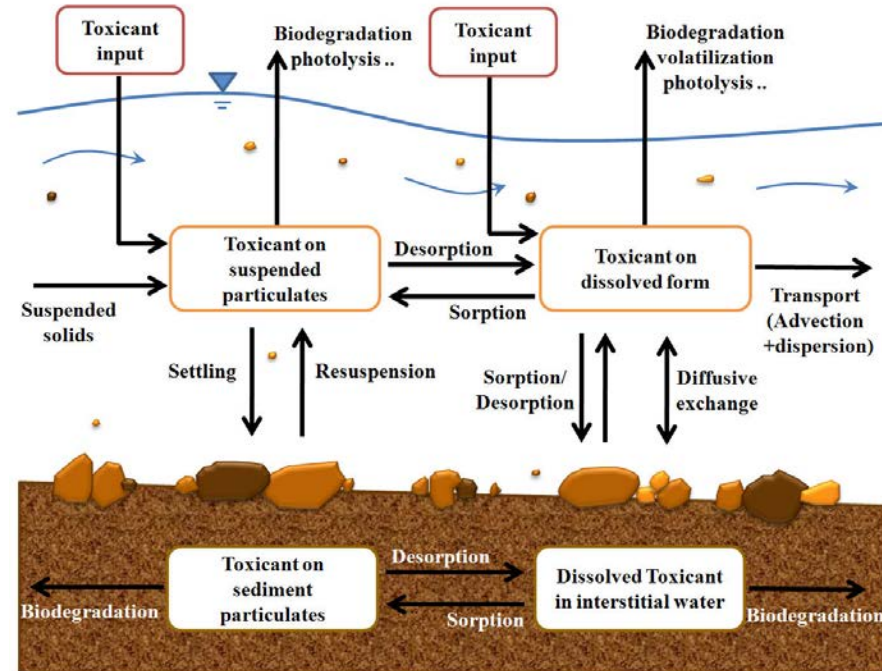


Chapter 6

River Water Quality Modeling



Chapter 6 River Water Quality Modeling

Contents

- 6.1 Non-Conservative Pollutants
- 6.2 Modeling BOD-DO Coupled System
- 6.3 Modeling Heat Transport
- 6.4 Eutrophication

Objectives

- Classify non-conservative pollutants
- Present concept of water quality modeling
- Study BOD-DO coupled system in the river
- Study transport of heat and algae

6.1 Non-Conservative Pollutants

6.1.1 Category of Non-Conservative Pollutants

1) Toxic Substance

- Metals: mercury, cadmium, lead
- Industrial chemicals: toluene, benzenes, phenols, PCB
- Hydrocarbons: PAH (polycyclic aromatic hydrocarbons)
- Agricultural chemicals: pesticides, herbicides, DDT
- Radioactive substances

6.1 Non-Conservative Pollutants

- 2) BOD-DO coupled system
- 3) Temperature
- 4) Nutrients and eutrophication
- 5) Bacteria and pathogens
- 6) Oil

[Cf] Conservative pollutants

- one which does not undergo any chemical or biochemical changes in transport
- no loss due to chemical reactions or biochemical degradation
- salt, chloride, total dissolved solids, some metals

6.1 Non-Conservative Pollutants

6.1.2 Transport of Non-Conservative Pollutants

(1) Toxic Substance

Physio-chemical phases of the transport of toxic substances:

- loss of the chemical due to biodegradation, volatilization, photolysis, and other chemical and bio-chemical reactions
- sorption and desorption between dissolved and particulate forms in the water column and bed sediment
- settling and resuspension mechanisms of particulates between water column and bed sediment

6.1 Non-Conservative Pollutants

Assume only loss of the chemical

$$\frac{\partial(hC)}{\partial t} + \frac{\partial}{\partial x}(uCh) + \frac{\partial}{\partial y}(vCh) = \nabla \cdot (hD\nabla C) + hS$$

where S = sink/source term

Assume first-order decay

- decay rate is proportional to the amount of material present

$$\frac{dC}{dt} = -kC = S$$

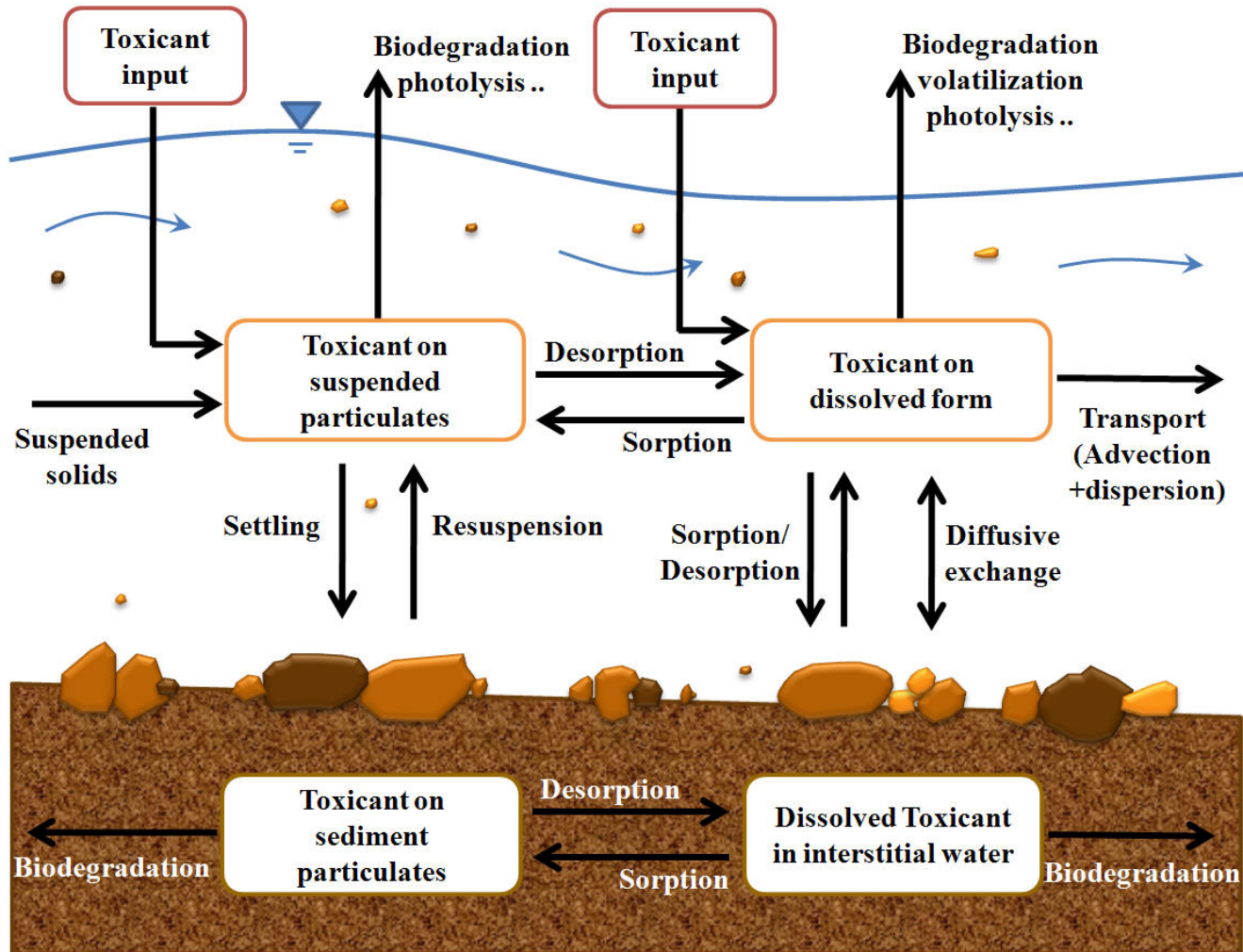
6.1 Non-Conservative Pollutants

where C = mass/volume; S = mass/(volume·time); k = 1/time = decay rate

- Rate of disappearance of BOD due to biodegradation
- Radioactive substance also decay in strength in this way
- Coliform bacteria and pathogens die away with a rate of first-order decay

$$\frac{\partial(hC)}{\partial t} + \frac{\partial}{\partial x}(uCh) + \frac{\partial}{\partial y}(vCh) = \nabla \cdot (hD\nabla C) - khC$$

6.1 Non-Conservative Pollutants

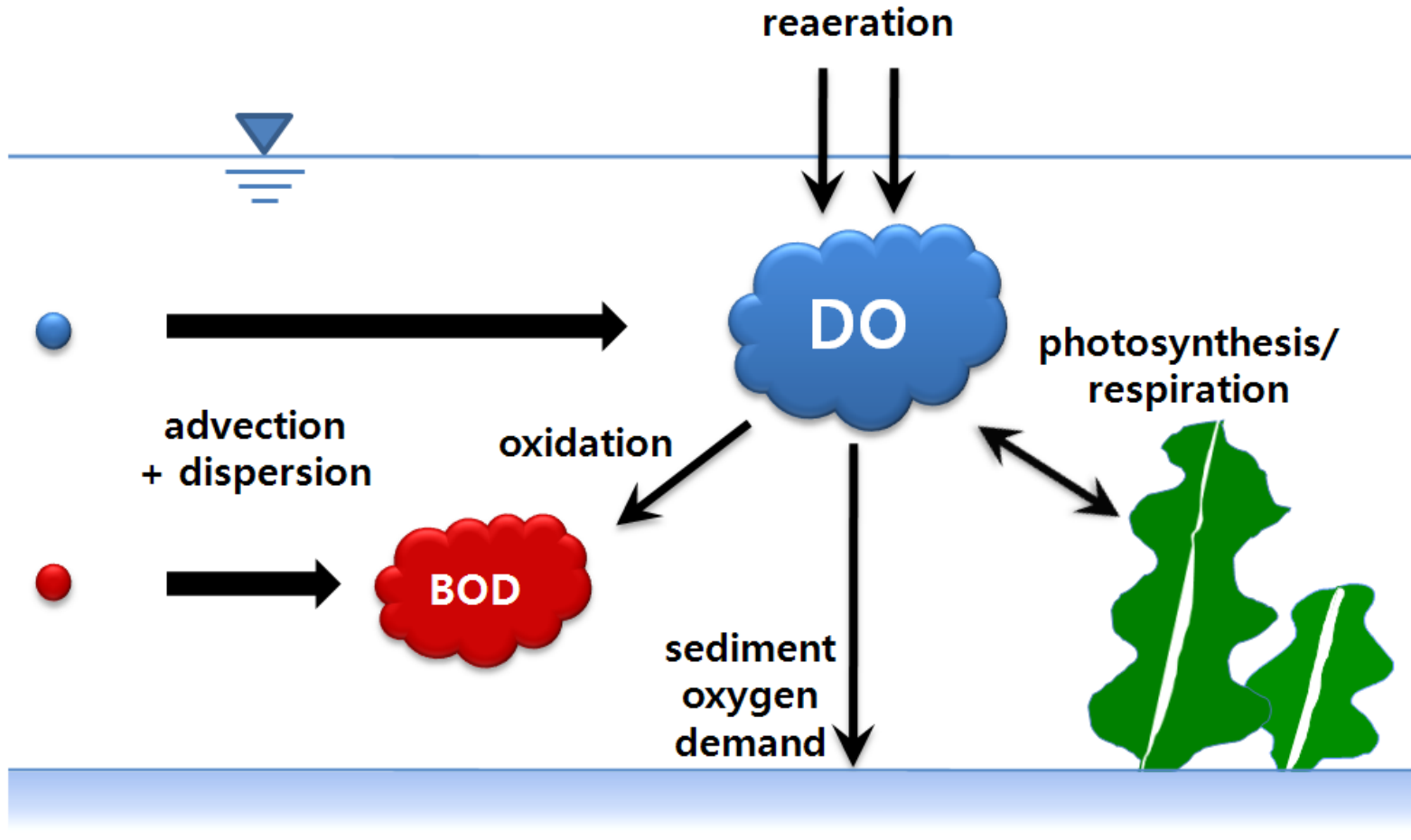


6.1 Non-Conservative Pollutants

(2) BOD-DO

- Linked materials
- Behavior of one material depends upon the amount of another- Conc. of dissolved oxygen depends not only on transport of DO but also on the amount of BOD present
- Biodegradable substances undergo biochemical reactions
- Oxygen is used up in aerobic decomposition

6.1 Non-Conservative Pollutants



6.1 Non-Conservative Pollutants

(3) Heat transport

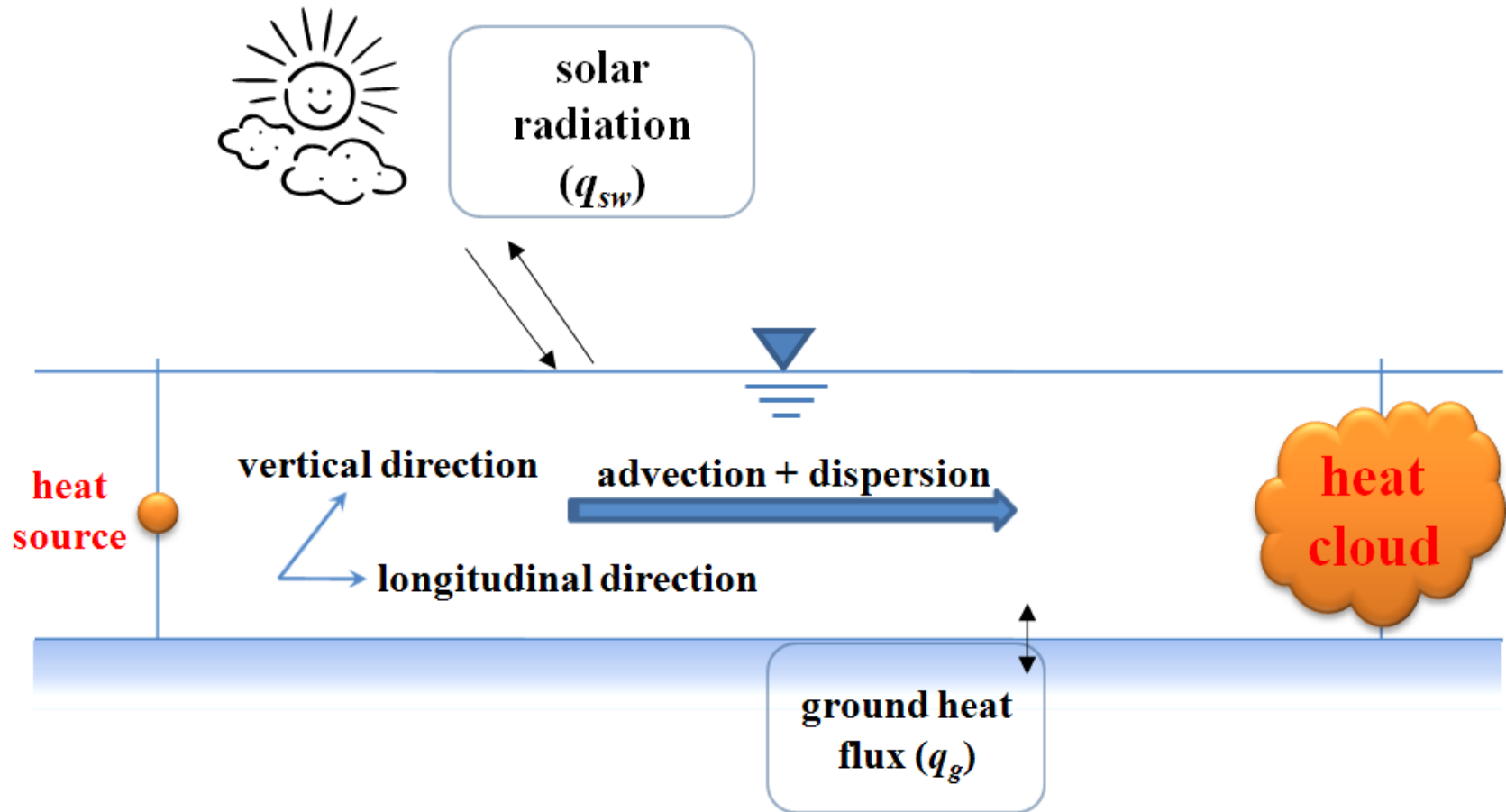
Heat and temperature

- Heat is the extensive quantity whereas temperature is intensive
(ex. Mass is the extensive property whereas concentration is intensive
(size-independent))
- Discharge of excess heat from industrial or municipal effluents may positively or negatively affect the aquatic ecosystem
- Strong influence many physiological and biochemical processes
- Control of the rate of biological and chemical reactions
- Oxygen solubility governed by water temperature (the colder the water, the more the dissolved oxygen)

6.1 Non-Conservative Pollutants

The heat exchange with the sediment bed is generally much smaller than the surface exchange and is frequently neglected in modeling studies (Morin and Couillard (1990), Hondzo and Stefan (1994), Younus et al. (2000)).

6.1 Non-Conservative Pollutants

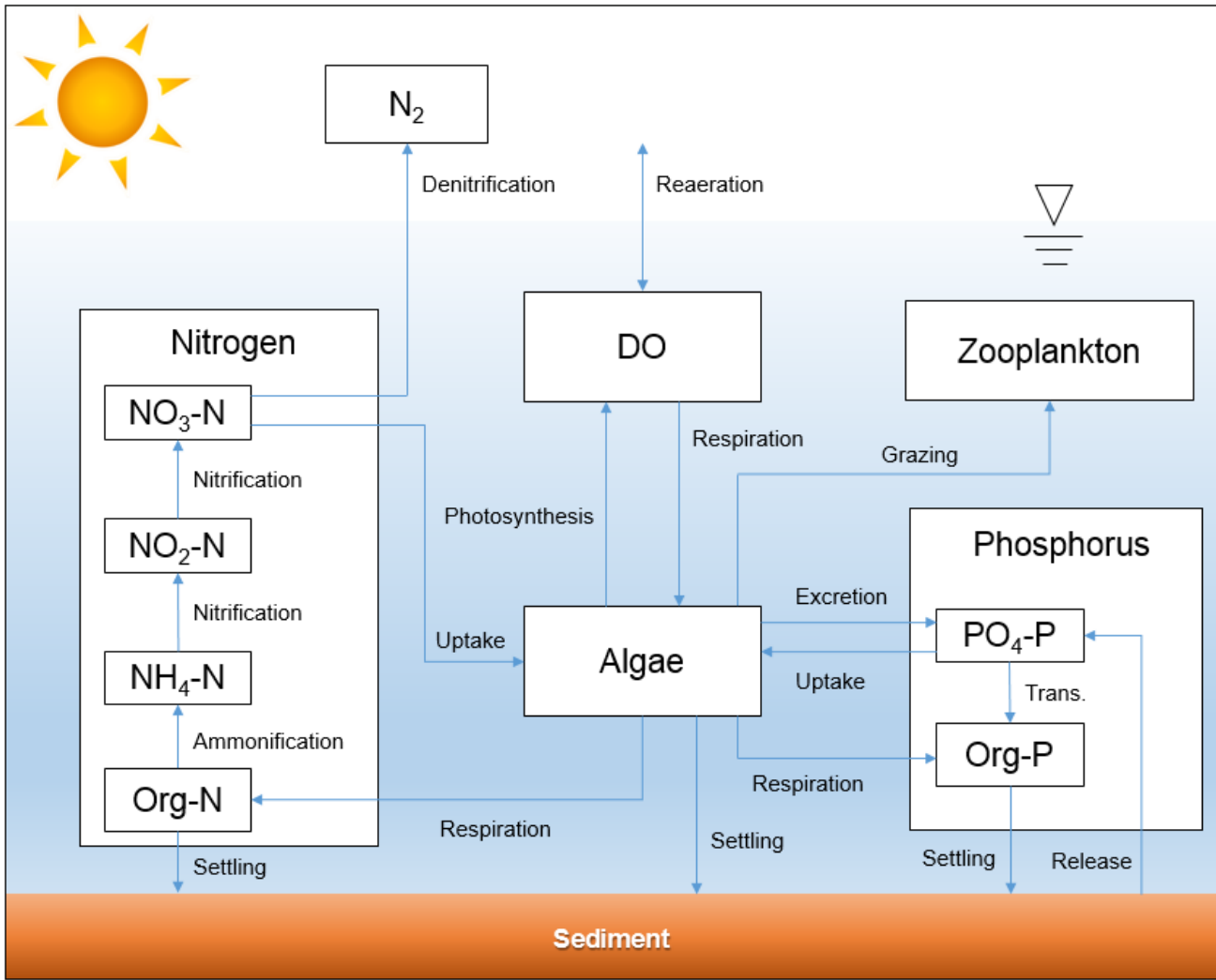


6.1 Non-Conservative Pollutants

(4) Eutrophication

- Eutrophication is excessive nutrients such as nitrogen and phosphorus in ecosystems.
- One example is algal bloom by great increase of algae.
- Adverse environmental effects involve the depletion of oxygen in the water bodies which cause a reduction in aquatic animals with water quality deterioration.
- Nitrogen and phosphorus are crucial indicators to assess eutrophication level.
- Algae and nutrients are transported by advection and dispersion with complex physicochemical processes.

6.1 Non-Conservative Pollutants



6.1 Non-Conservative Pollutants

(5) Bacteria and Pathogens

- Related to waterborne diseases (e.g., gastroenteritis, amoebic dysentery, cholera, etc.)
- The modes of transmission of pathogens are through drinking water, primary & secondary contact recreation, etc.
- Examples of communicable disease indicators and pathogens

6.1 Non-Conservative Pollutants

Type	Organisms
Indicator bacteria	Total Coliform, Fecal Coliform, E. Coli, Fecal streptococci, Enterococci, etc.
Pathogens	Vibrio cholera, Salmonella species, Shigella species, Giardia lamblia, Entamoeba histolytica, etc.

6.1 Non-Conservative Pollutants

- The principal sources of organisms:
 - (a) point sources from domestic, municipal, and some industrial sources
 - (b) combined sewer overflows
 - (c) runoff from urban and suburban land
 - (d) municipal waste sludges disposed of on land or in water bodies

- Decay rate

$$K_B = K_{B1} + K_{BI} + K_{Bs} - K_a$$

6.1 Non-Conservative Pollutants

where, K_{B1} = basic death rate as a function of temperature, salinity, predation,

K_{BI} = death rate due to sunlight, K_a = net loss due to settling (resuspension)

K_{Bs} = after growth rate

- For rivers and streams, the downstream distribution of bacteria is

$$N = N_0 \exp(-K_B t^*)$$

where, N_0 = the concentration at the outfall after mixing [num/L³],

K_B = the overall net first-order decay rate [1/day], $t^* = x / U$

6.1 Non-Conservative Pollutants

(6) Oil

i) Advection

- Advection of oil is recognized as a three-dimensional process, with key mechanisms occurring over a wide range of scales
- Oil moves horizontally in the water under forcing from wind, waves and currents
- Transported vertically in the water column in the form of droplets of various sizes

6.1 Non-Conservative Pollutants

ii) Spreading

- Oil film thickness determines the persistence of the oil on the water surface
- Oil slick area (film thickness) is used in the computation of evaporation, which determines changes in oil composition and properties with time
- For instantaneous spills, Fay-type spreading model (Fay, 1971) provides adequate predictions of the film thickness

6.1 Non-Conservative Pollutants

$$A \sim \left(\frac{\sigma^2 V^6}{\rho^2 \nu D^3 s^6} \right)^{1/8}$$

where σ = spreading coefficient or interfacial tension, V = volume of oil in axisymmetric spread, ρ = density of water, ν = kinematic viscosity of water, D = diffusivity of the surfactants in water, s = solubility

iii) Evaporation

- Estimates of evaporative losses are required in order to assess the persistence of the spill, and are also the basis for estimates of changes in oil properties with time

6.1 Non-Conservative Pollutants

- During a spill, approximately 25 ~ 40% of the total mass can be lost by evaporation alone, depending on the environmental conditions and the type of oil (Azevedo *et al.*, 2014)
- Evaporative exposure formulation (Stiver and Mackay, 1984)

$$\frac{dF_v}{dt} = \frac{K_e A}{V_0} \exp \left[6.3 - \frac{10.3}{T} (T_0 + T_G F_v) \right]$$

where F_v = fraction evaporated, t = time, $K_e = 2.0 \times 10^{-3} \times U_w^{0.78}$, U_w = wind velocity, A = film thickness, T = environmental temperature (K), T_0 and T_G = oil-dependent parameters derived from the fractional distillation data

6.1 Non-Conservative Pollutants

iv) Natural dispersion

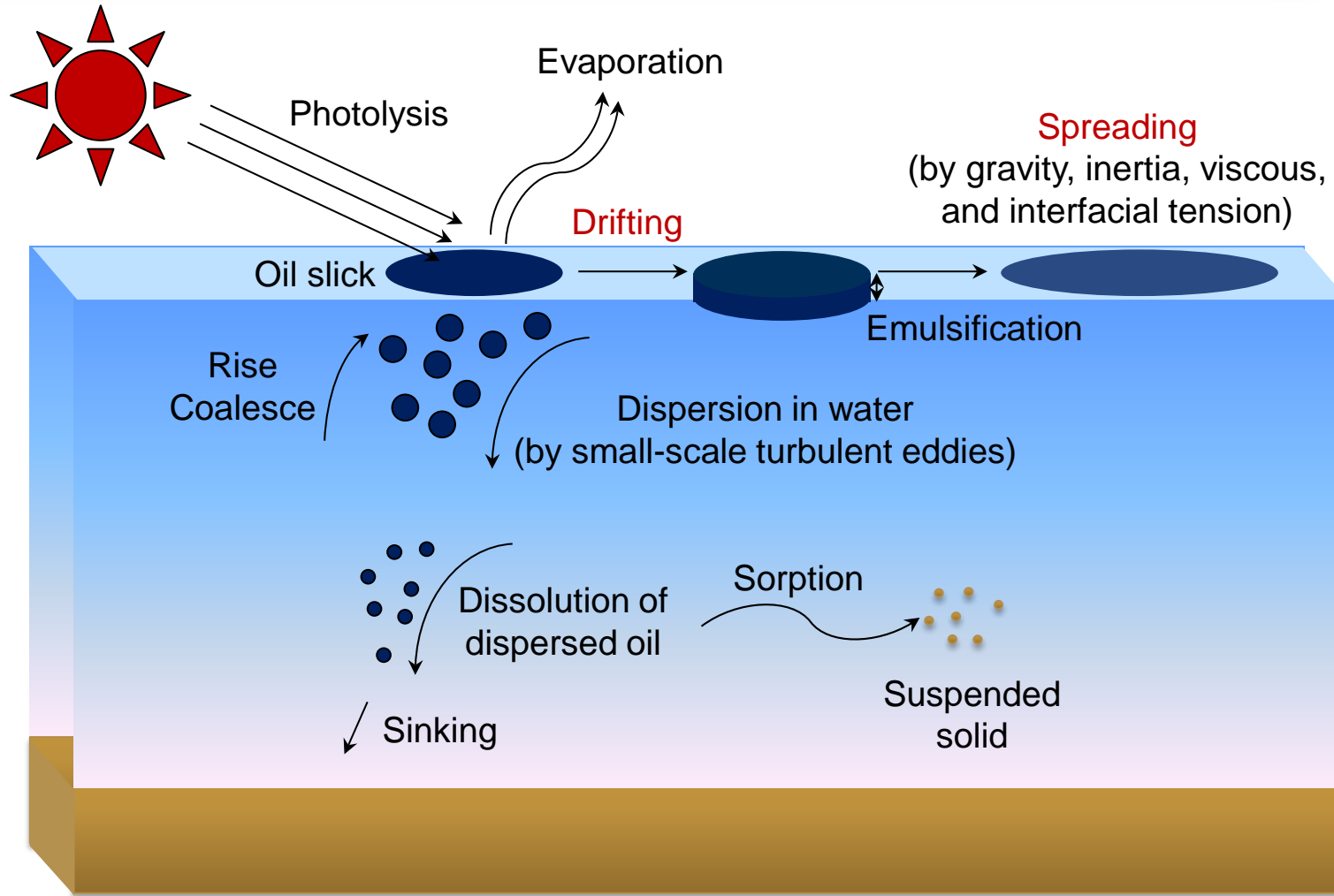
- Computation of natural dispersion is required for assessment of lifetime of an oil spill
- The rate of natural dispersion depends on environmental parameters, but is also influenced by oil-related parameters (oil film thickness, density, surface tension and viscosity)
- Experimental work of Delvigne and Sweeny (1988) revealed that the number of droplets in a certain diameter class could be related to the droplet size with a common power law relationship, independent of the type of oil and the wave conditions

6.1 Non-Conservative Pollutants

$$Q_{d \leq D} = aH^{1.4} D^{1.7}$$

where $Q_{d \leq D}$ = entrained oil mass per unit area included in droplets up to a certain diameter D , a = dispersion coefficient which is related to the oil type in terms of the oil viscosity, H = breaking wave height

6.1 Non-Conservative Pollutants



6.2 Modeling BOD-DO Coupled System

6.2.1 Solutions of BOD-DO Coupled System

- ◆ Coupled system (BOD, DO)

- determination of dissolved oxygen concentrations downstream of a discharge of BOD

- ◆ Oxygen Demand

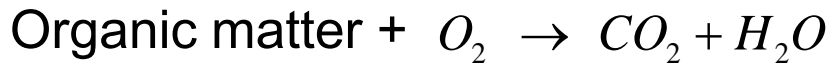
- = indirect measure of organic materials (= organic pollutants) in terms of the amount of oxygen required to (completely) oxidize it.

6.2 Modeling BOD-DO Coupled System

COD - Chemical Oxygen Demand

BOD: CBOD - Carbonaceous BOD

NBOD - Nitrogenous BOD



◆ Importance of dissolved oxygen (DO)

- Anaerobic conditions in a stream are indicative of extreme pollution
- Low dissolved oxygen concentrations have severe effects on the kind of biota which inhabit the stream

6.2 Modeling BOD-DO Coupled System

◆ Sources and sinks of DO

(a) Sources

- Reaeration from the atmosphere
- Photosynthetic oxygen production
- DO in incoming tributaries

(b) Sinks

- Oxidation of BOD
- Oxygen demand of sediments of water body
- Use of oxygen for respiration by aquatic plants

6.2 Modeling BOD-DO Coupled System

$$\therefore \frac{dC}{dt} = \text{reaeration} + (\text{Photosynthesis-respiration}) - \text{oxydation of BOD}$$

– sediment oxygen demand \pm oxygen transport (into and out of segment)

Let C = concentration of DO

L = concentration of BOD

(1) rate of utilization of DO by BOD

$$\frac{dL}{dt} = -k_1 L \rightarrow \text{exertion of BOD}$$

= utilization of DO

= depletion of DO

k_1 = deoxygenation coefficient

6.2 Modeling BOD-DO Coupled System

(2) reaeration from the atmosphere

= diffuse of oxygen into the stream rate of reaeration

\propto degree to which the water is unsaturated with oxygen

Let C_s = DO saturation concentration

then oxygen deficit, $DOD = C_s - C$

\therefore rate of reaeration

$$\frac{dC}{dt} = +k_2(C_s - C)$$

k_2 = reaeration coefficient (1/T)

6.2 Modeling BOD-DO Coupled System

∴ Conservation equation for C

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E \frac{\partial^2 C}{\partial x^2} - k_1 L + k_2 (C_s - C)$$

Let

$$D = C_s - C$$

Then

$$dD = -dC$$

$$\therefore -\frac{\partial D}{\partial t} = +u \frac{\partial D}{\partial x} - E \frac{\partial^2 D}{\partial x^2} - k_1 L + k_2 D$$

$$\frac{\partial D}{\partial t} = -u \frac{\partial D}{\partial x} + E \frac{\partial^2 D}{\partial x^2} + k_1 L - k_2 D \Rightarrow \text{G.E. for DO Deficit}$$

6.2 Modeling BOD-DO Coupled System

For BOD

$$\frac{\partial L}{\partial t} = -u \frac{\partial L}{\partial x} + E \frac{\partial^2 L}{\partial x^2} - k_1 L \Rightarrow \text{G.E. for BOD concentration}$$

Let reaction terms

$$S_L = -k_r L$$

$$S_D = k_d L - k_a D$$

in which

L = concentration of remaining BOD

D = dissolved oxygen deficit (DOD) = $C_s - C$

6.2 Modeling BOD-DO Coupled System

C_s = DO saturation concentration

C = actual DO concentration

k_r = BOD removal coefficient = $k_d + k_s$

k_s = settling coefficient

k_d = deoxygenation coefficient = biochemical degradation

k_a = reaeration coefficient

6.2 Modeling BOD-DO Coupled System

G.E.: unsteady state

$$\text{BOD} \quad \frac{\partial L}{\partial t} = -u \frac{\partial L}{\partial x} + E \frac{\partial^2 L}{\partial x^2} - k_r L$$

$$\text{DOD} \quad \frac{\partial D}{\partial t} = -u \frac{\partial D}{\partial x} + E \frac{\partial^2 D}{\partial x^2} + k_d L - k_a D$$

◆ Steady state, W/ Dispersion (Estuary)

(i) BOD: $0 = -u \frac{\partial L}{\partial x} + E \frac{\partial^2 L}{\partial x^2} - k_r L \rightarrow$ same as case 4

$$L = L_0 \exp \left[\frac{u}{2E} (1 + \alpha_r) x \right], \quad x \leq 0$$

$$= L_0 \exp \left[\frac{u}{2E} (1 - \alpha_r) x \right], \quad x \leq 0$$

6.2 Modeling BOD-DO Coupled System

in which

$$L_0 = \frac{W}{Q\alpha_r}$$

$$\alpha_r = \sqrt{1 + \frac{4k_r E}{u^2}}$$

(ii) DO: $0 = -u \frac{\partial D}{\partial x} + E \frac{\partial^2 D}{\partial x^2} + k_d L - k_a D$

$$D = \frac{W}{Q} \frac{k_d}{k_a - k_r} \left\{ \frac{\exp\left[\frac{u}{2E}(1 + \alpha_r)x\right]}{\alpha_r} - \frac{\exp\left[\frac{u}{2E}(1 - \alpha_a)x\right]}{\alpha_a} \right\}, \quad x \leq 0$$

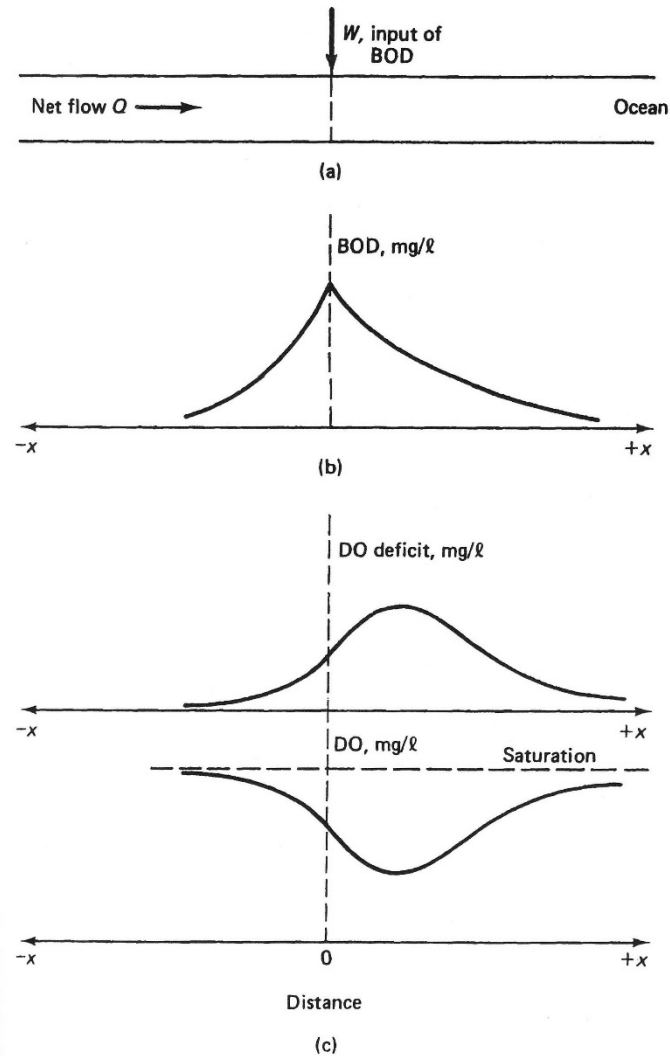
$$D = \frac{W}{Q} \frac{k_d}{k_a - k_r} \left\{ \frac{\exp\left[\frac{u}{2E}(1 - \alpha_r)x\right]}{\alpha_r} - \frac{\exp\left[\frac{u}{2E}(1 + \alpha_a)x\right]}{\alpha_a} \right\}, \quad x \geq 0$$

6.2 Modeling BOD-DO Coupled System

in which

$$\alpha_a = \sqrt{1 + \frac{4k_a E}{u^2}}$$

6.2 Modeling BOD-DO Coupled System



6.2 Modeling BOD-DO Coupled System

6.2.2 Streeter-Phelps Equation

◆ Streeter-Phelps Equation (1925)

- no dispersion (river) $E = 0$

- steady state

$$\text{BOD: } 0 = -u \frac{\partial L}{\partial x} - k_1 L$$

$$\text{DO: } 0 = -u \frac{\partial D}{\partial x} + k_1 L - k_2 D$$

6.2 Modeling BOD-DO Coupled System

For BOD we have solution (Case 3)

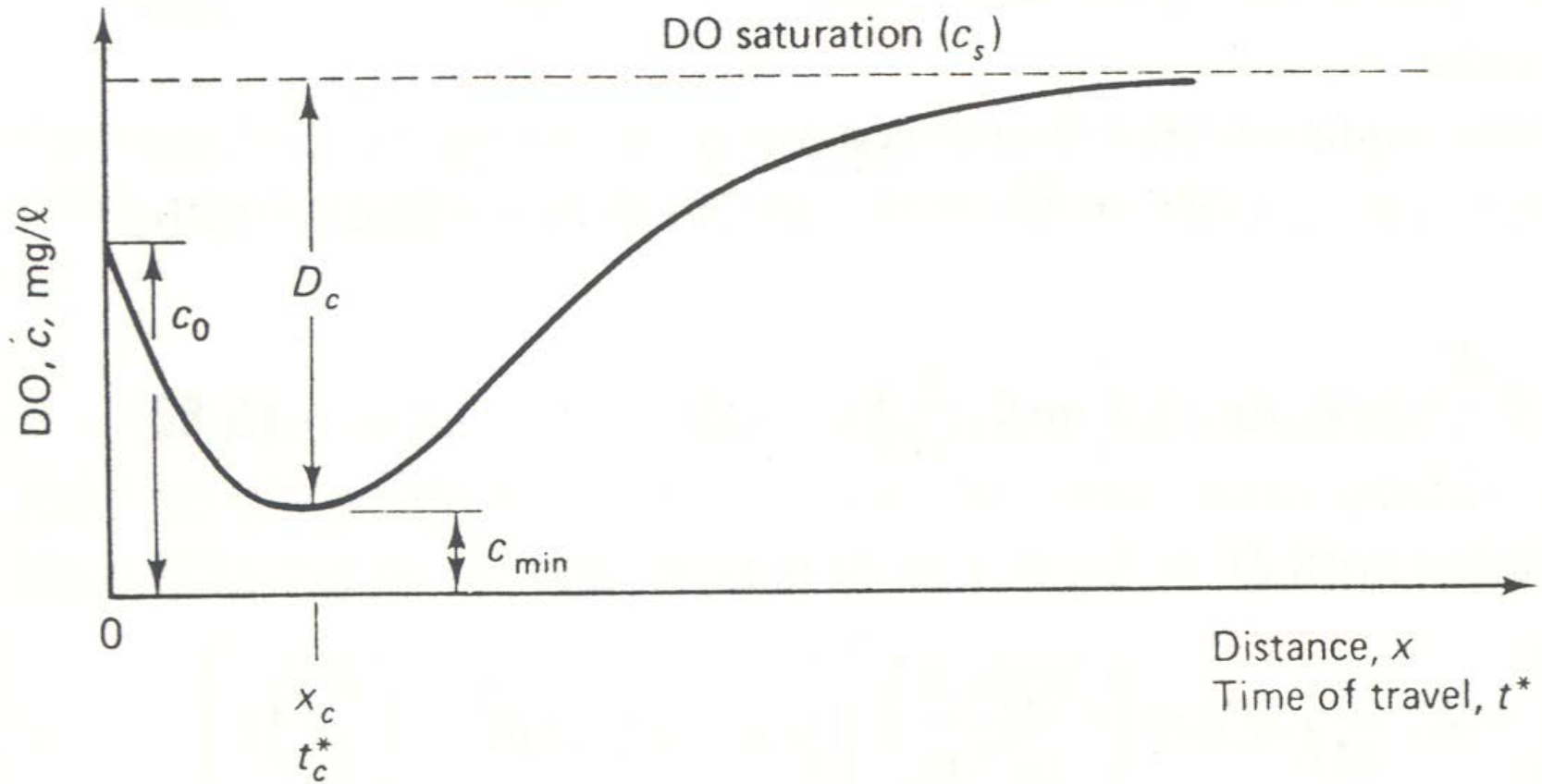
$$\therefore L = L_0 \exp\left(-\frac{k_1}{u}x\right) = \frac{W}{Q} \exp\left(-\frac{k_1}{u}x\right)$$

$$\text{B.C.: } D(0) = D_0 = C_s - C_0$$

Solution:

$$D(x) = \frac{k_1}{k_2 - k_1} L_0 \left[e^{-\left(\frac{k_1}{u}\right)x} - e^{-\left(\frac{k_2}{u}\right)x} \right] + D_0 e^{-\left(\frac{k_2}{u}\right)x}, \quad x \geq 0 \quad (1)$$

6.2 Modeling BOD-DO Coupled System



6.2 Modeling BOD-DO Coupled System

- ◆ Critical deficit D_c (@ t_c uptake of oxygen by BOD is just balanced by the input of oxygen from atmosphere)

let $x/u = t$ (= time of flow) time of travel

→ Then Eq. (1) becomes

$$D(t) = \frac{k_1}{k_2 - k_1} L_0 \left[e^{-k_1 t} - e^{-k_2 t} \right] + D_0 e^{-k_2 t}, \quad x \geq 0 \quad (2)$$

6.2 Modeling BOD-DO Coupled System

→ t_c may be found as

$$\frac{\partial D}{\partial t} = 0; \quad t_c = \frac{1}{k_2 - k_1} \ln \left\{ \frac{k_2}{k_1} \left[1 - \frac{(k_2 - k_1) D_0}{L_0} \right] \right\}$$

$$D_c = \frac{k_1}{k_2} L_0 e^{-k_1 t_c} \quad \leftarrow \text{from Eq.(2)}$$

- ◆ Modified Streeter-Phelps equation
- account for other processes

6.2 Modeling BOD-DO Coupled System

(1) BOD removal due to sedimentation

- non-oxygen-demanding
- reduces BOD w/o changing oxygen concentration

$$\frac{\partial L}{\partial t} = -k_3 L$$

(2) BOD addition due to scour from the bottom and surface runoff from the land

- rate of addition is assumed to be constant

(3) Oxygen use other than by aerobic biochemical oxygen demand in the water, and oxygen addition other than through reaeration.

- net of these processes is constant rate A

6.2 Modeling BOD-DO Coupled System

◆ Solution :

$$D_t = \frac{k_1}{k_2 - (k_1 + k_3)} \left(L_0 - \frac{P}{k_1 + k_2} \right) \left\{ e^{-(k_1 + k_2)t} - e^{-k_2 t} \right\} \\ + \frac{k_1}{k_2} \left(\frac{P}{k_1 + k_2} - \frac{A}{k_1} \right) (1 - e^{-k_2 t})$$

Consider only k_3 neglect A & P

Let $k_r = k_1 + k_3$, $k_d = k_1$, $k_s = k_3$, $k_a = k_2$

Then

$$D_t = \frac{k_d}{k_a - k_r} L_0 \left\{ e^{-k_r t} - e^{-k_a t} \right\} + D_0 e^{-k_a t}$$

6.2 Modeling BOD-DO Coupled System

[Remark]

$$\text{G.E.: } 0 = -u \frac{\partial L}{\partial x} - k_r L \quad \text{BOD}$$

$$0 = -u \frac{\partial D}{\partial x} + k_d L - k_a D \quad \text{DOD}$$

6.3 Modeling Heat Transport

◆ Sources and sinks of heat

(a) Sources

- Shortwave solar radiation
- Longwave atmospheric radiation
- Conduction of heat from atmosphere to water
- Direct heat input from municipal and industrial activities

(b) Sinks (losses)

- Longwave radiation emitted by water
- Evaporation
- Conduction from water to atmosphere

6.3 Modeling Heat Transport

- ◆ Heat balance equation

Edinger and Geyer (1965) and Edinger et al. (1974) provide a review of each of the process.

$$q_{net} = q_s + q_a + q_b + q_c + q_e$$

where

q_{net} = net heat exchange across the water surface

q_s = shortwave solar radiation

q_a = longwave atmospheric radiation

q_b = longwave radiation from water

q_e = conductive heat transfer

q_c = evaporative heat transfer

6.3 Modeling Heat Transport

All terms are in units such as. $\text{cal/cm}^2 \cdot \text{day}$

◆ Simplified heat balance equation

Edinger et al. (1974) have shown that the net heat input can be represented by

$$q_{net} = K(T_e - T)$$

where

K = surface heat exchange coefficient ($\text{W/m}^2\text{°C}$)

T_e = equilibrium temperature

= temperature that a body of water would reach if all meteorological conditions were constant in time

6.3 Modeling Heat Transport

- ◆ Exchange coefficient, K

Edinger et al. (1974) proposed as follows,

$$K = 4.5 + 0.05T + \beta f(U_w) + 0.47 f(U_w)$$

where

$$f(U_w) = 9.2 + 0.46U_w^2 = \text{wind function (W/m}^2 \cdot \text{mm Hg)}$$

U_w = wind speed in m/s (measured at a height of 7 m above the water surface)

$$\beta = 0.35 + 0.015T_m + 0.0012T_m^2$$

$$T_m = (T + T_d) / 2$$

T_d = dew point temperature

6.3 Modeling Heat Transport

- ◆ Equilibrium temperature, T_e

The equilibrium temperature can be estimated for a given set of meteorological conditions by iteration until $q_{net} = 0$. Alternately, under constant coefficients, the equilibrium temperature as given by Edinger et al. (1974), is approximated by the empirical relationship

$$T_e = T_d + \frac{q_s}{K}$$

- ◆ Time rate of change of temperature

$$\frac{dT}{dt} = \frac{q_{net}}{\rho c_p h} = \frac{K(T_e - T)}{\rho c_p h}$$

6.3 Modeling Heat Transport

where

ρ = water density (g/cm³)

C_p = specific heat of water (1 cal/g°C)

◆ Heat transport equation

$$\frac{\partial hT}{\partial t} + \frac{\partial}{\partial x}(uTh) + \frac{\partial}{\partial y}(vTh) = \nabla \cdot (hD\nabla T) + hS$$

$$S = \frac{dT}{dt} = \frac{q_{net}}{\rho c_p h} = \frac{K(T - T_e)}{\rho c_p h}$$

Assume that u, v, h satisfy the continuity eq.

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{1}{h} \nabla \cdot (hD\nabla T) + \frac{K}{\rho c_p} (T_e - T)$$

6.4 Eutrophication

6.4.1 Modeling Nitrogen and Phosphorus

- ◆ Transport of nitrogen and phosphorus
 - Advection and dispersion are the most important mechanisms in the nutrient transport
 - Nutrients involve chemical reactions or biological evolutions
 - General partial differential equation of nutrients for a one-dimensional model:

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E \frac{\partial^2 C}{\partial x^2} \pm S - kC$$

6.4 Eutrophication

where

C = concentration of nutrients

E = longitudinal dispersion coefficient

S = sink and source by external contribution

k = first-order decay

Let $\pm S - kC = R(C, t)$

$$\therefore \frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E \frac{\partial^2 C}{\partial x^2} + R(C, t)$$

where

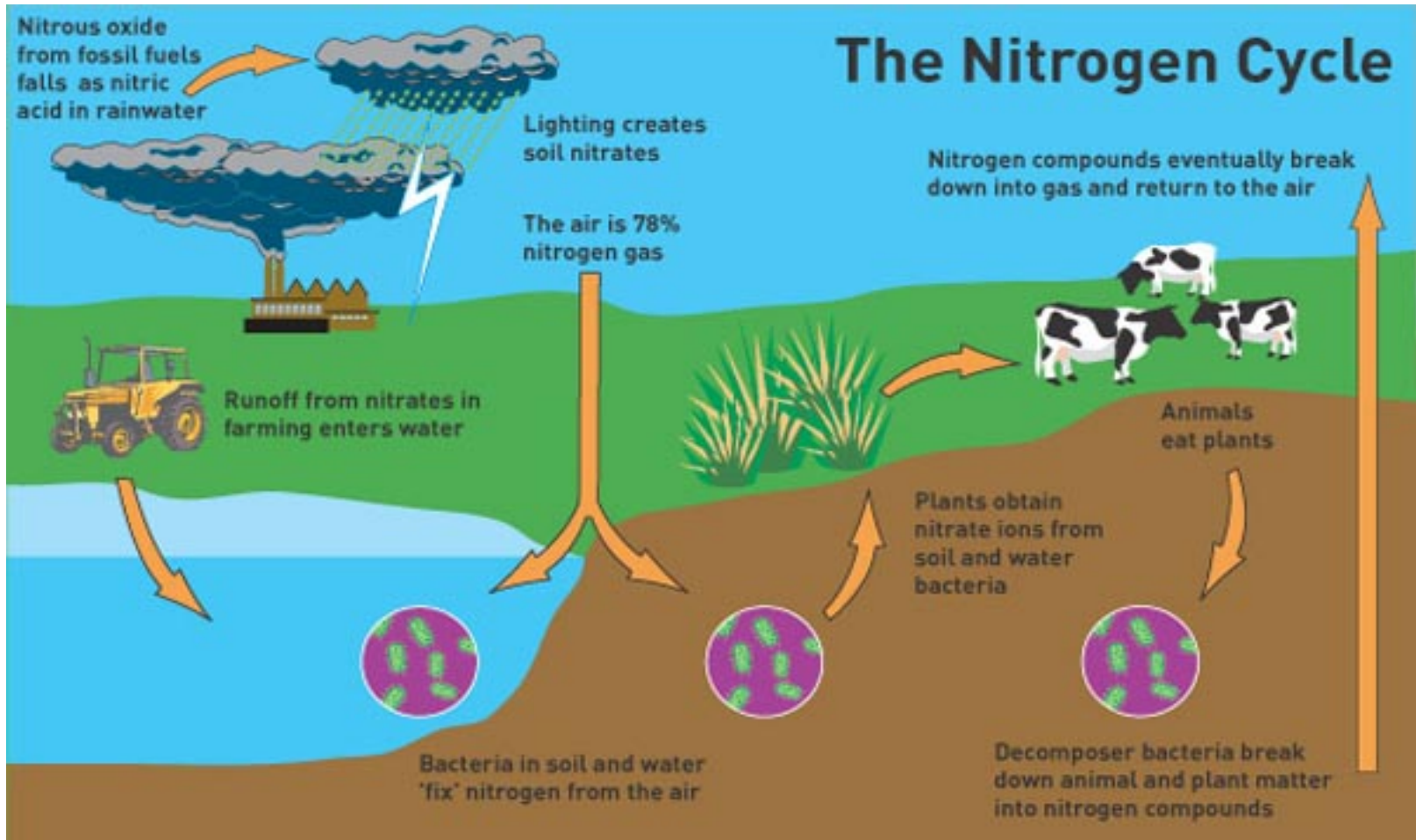
$R(C, t)$ = reaction term of nutrients

6.4 Eutrophication

◆ Nitrogen cycle

- The primary source of nitrogen is agricultural soil management with synthetic fertilizers, accounting for about 74% of total NO_2 emission in 2013 (USEPA, 2015).
- The nitrogen cycle considers ammonia nitrogen ($\text{NH}_4\text{-N}$), nitrite nitrogen ($\text{NO}_2\text{-N}$), nitrate nitrogen ($\text{NO}_3\text{-N}$), and organic nitrogen (Org-N).
- Nitrification and denitrification are important phases in the nitrogen cycle

6.4 Eutrophication



6.4 Eutrophication

◆ Reaction terms of nitrogen

(1) organic nitrogen (Org-N)

- Source: respiration by algae
- Decay: ammonification from organic nitrogen to ammonia nitrogen, and settling
- Ammonification: $Org-N + 3H_2O \rightarrow 2NH_4^+ + HCO_3^- + OH^-$

$\therefore R(N_{org}, t) = \text{respiration} - \text{ammonification} - \text{settling}$

$$= \alpha_{n,A} k_{r,A} \theta_A^{(T-20)} A - \left(k_{n,org} \theta_{n,org}^{(T-20)} + \frac{\omega_{n,org}}{h} \right) N_{org}$$

6.4 Eutrophication

where

N_{org} = concentration of organic nitrogen

$\alpha_{n,A}$ = nitrogen content in algae

$k_{r,A}$ = algal respiration rate

θ_A = temperature coefficient for algae

$\theta_{n,org}$ = temperature coefficient for organic nitrogen

T = water temperature

A = concentration of algae

$k_{n,org}$ = rate of ammonification of organic nitrogen into ammonia nitrogen

$\omega_{n,org}$ = rate of organic nitrogen settling

h = water depth

6.4 Eutrophication

(2) ammonia-nitrogen ($\text{NH}_4\text{-N}$)

- Source: ammonification from organic nitrogen to ammonia-nitrogen
- Decay: nitrification from ammonia-nitrogen to nitrite-nitrogen
- Nitrification (a): $\text{NH}_4^+ + 1.5\text{O}_2 \rightarrow \text{NO}_2^- + \text{H}_2\text{O} + 2\text{H}^+$

$$\therefore R(N_{amm}, t) = \text{ammonification} - \text{nitrification (a)}$$

$$= k_{n,org} \theta_{n,org}^{(T-20)} N_{org} - k_{n,amm} \theta_{n,amm}^{(T-20)} N_{amm}$$

6.4 Eutrophication

where

N_{amm} = concentration of ammonia-nitrogen

$k_{n,amm}$ = nitrification rate of ammonia-nitrogen into nitrite-nitrogen

$\theta_{n,amm}$ = temperature coefficient for ammonia-nitrogen

(3) nitrite-nitrogen ($\text{NO}_2\text{-N}$)

- Source: nitrification from ammonia-nitrogen to nitrite-nitrogen
- Decay: nitrification from nitrite-nitrogen to nitrate-nitrogen

Nitrification (b): $\text{NO}_2^- + 0.5\text{O}_2 \rightarrow \text{NO}_3^-$

6.4 Eutrophication

$$\begin{aligned} \therefore R(N_{nitri}, t) &= \text{nitrification (a)} - \text{nitrification (b)} \\ &= k_{n,amm} \theta_{n,amm}^{(T-20)} N_{amm} - k_{n,nitri} \theta_{n,nitri}^{(T-20)} N_{nitri} \end{aligned}$$

where

N_{nitri} = concentration of nitrite-nitrogen

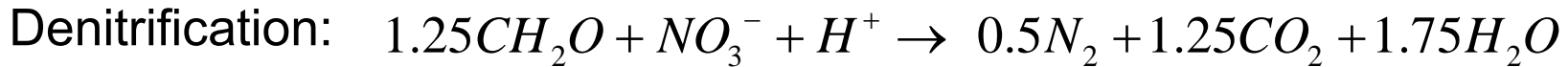
$k_{n,nitri}$ = nitrification rate of nitrite-nitrogen into nitrate-nitrogen

$\theta_{n,nitri}$ = temperature coefficient for nitrite-nitrogen

6.4 Eutrophication

(4) nitrate-nitrogen ($\text{NO}_3\text{-N}$)

- Source: nitrification from nitrite-nitrogen to nitrate-nitrogen
- Sink: uptake by algae
- Decay: denitrification from nitrate-nitrogen to nitrogen gas (N_2)



$$\therefore R(N_{\text{nitra}}, t) = \text{nitrification (b)} - \text{denitrification} - \text{uptake}$$

$$= k_{n,\text{nitri}} \theta_{n,\text{nitri}}^{(T-20)} N_{\text{nitri}} - k_{n,\text{nitra}} \theta_{n,\text{nitra}}^{(T-20)} N_{\text{nitra}} - \alpha_{n,A} \mu A$$

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where

N_{nitra} = concentration of nitrate-nitrogen

$k_{n,nitra}$ = denitrification rate of nitrate-nitrogen into nitrogen gas

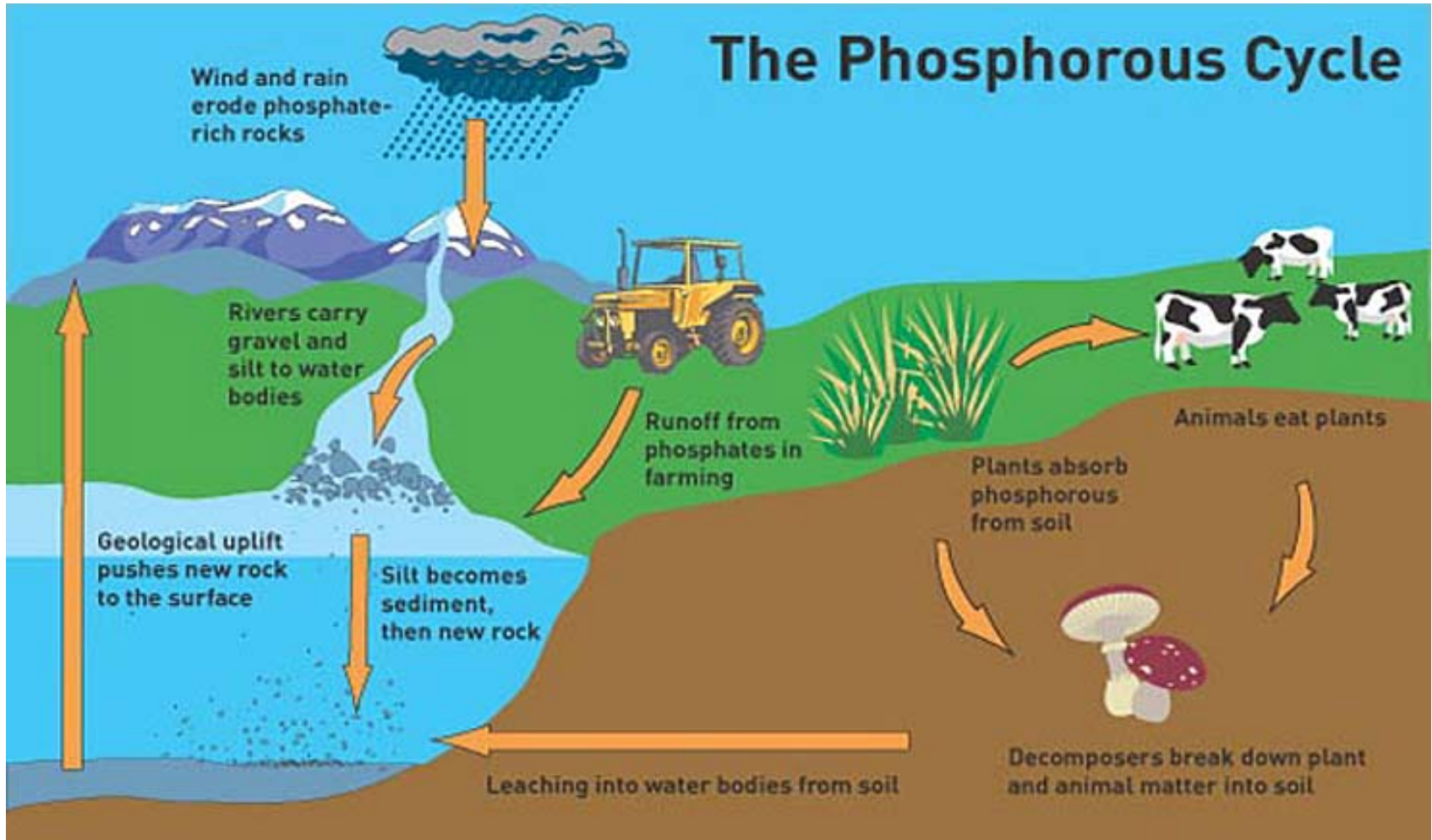
$\theta_{n,nitra}$ = temperature coefficient for nitrate-nitrogen

μ = algal growth rate

◆ Phosphorus Cycle

- The phosphorus cycle has no major gaseous component.
- Phosphorus loading contributed by runoff from pastures and croplands with livestock waste and fertilizers (USGS, 2000)
- The phosphorus cycle includes organic phosphorus (Org-P), and dissolved phosphorus or phosphate phosphorus (PO_4 -P).

6.4 Eutrophication



6.4 Eutrophication

◆ Reaction terms of phosphorus

(1) organic phosphorus (Org-P)

- Source: respiration by algae
- Decay: mineralization from organic phosphorus to phosphate-phosphorus, and settling

-

$\therefore R(P_{org}, t)$ = respiration – mineralization – settling

$$= \alpha_{p,A} k_{r,A} \theta_A^{(T-20)} A - \left(k_{p,org} \theta_{p,org}^{(T-20)} + \frac{\omega_{p,org}}{h} \right) P_{org}$$

6.4 Eutrophication

where

P_{org} = concentration of organic phosphorus

$\alpha_{p,A}$ = phosphorus content in algae

$k_{p,org}$ = mineralization of organic phosphorus into phosphate phosphorus

$\theta_{p,org}$ = temperature coefficient for organic phosphorus

$\omega_{p,org}$ = rate of organic phosphorus settling

(2) phosphate-phosphorus ($\text{PO}_4\text{-P}$)

- Source: mineralization, excretion from algae, and aerobic release from sediment
- Sink: uptake by algae

6.4 Eutrophication

$\therefore R(P_{diss}, t) = \text{mineralization} + \text{excretion} + \text{release} - \text{uptake}$

$$= k_{p,org} \theta_{p,org}^{(T-20)} P_{org} + \frac{\gamma_{p,diss}}{h} + \alpha_{p,A} \left(k_{e,A} \theta_A^{(T-20)} - \mu \right) A$$

where

P_{diss} = concentration of phosphate phosphorus

$\gamma_{p,diss}$ = rate of aerobic release from sediment

$k_{e,A}$ = algal excretion rate

6.4 Eutrophication

6.4.2 Modeling Algae

- ◆ Characteristics of algae
 - Aquatic photosynthesis micro-organisms
 - Diatom, green algae and cyanobacteria are common species in the water systems
 - The presence of algae in the river depends on the factors including: nutrients, temperature, and sunlight intensity (Hornbeger and Kelly, 1975; Zhen-Gang, 2008).
 - Coupled with nitrogen and phosphorus cycle

6.4 Eutrophication



6.4 Eutrophication

- ◆ Transport of algae
 - Similar to the nutrient transport
 - Growth rate is added instead of sink-source in the reaction term.
 - General partial differential equation of algae for a one-dimensional model:

$$\frac{\partial A}{\partial t} = -u \frac{\partial A}{\partial x} + E \frac{\partial^2 A}{\partial x^2} + \mu A - kA$$

Let $\mu A - kA = R(A, t)$

$$\therefore \frac{\partial A}{\partial t} = -u \frac{\partial A}{\partial x} + E \frac{\partial^2 A}{\partial x^2} + R(A, t)$$

where

$R(A, t)$ = reaction term of algae

6.4 Eutrophication

◆ Reaction term of algae

- Growth: photosynthesis (or uptake of nitrate nitrogen and phosphate phosphorus)
- Algal growth is a function of temperature, light, and nutrients (Bowie, 1985)
- Decay: respiration, excretion, grazing by zooplankton, and settling



$$\therefore R(A, t) = \left[\mu_{\max} \cdot f(T) \cdot f(N) \cdot f(I) - k_{r,A} \theta_A^{(T-20)} - k_{e,A} \theta_A^{(T-20)} - k_{z,A} \theta_A^{(T-20)} - \frac{\omega_A}{h} \right] A$$

6.4 Eutrophication

where

μ_{\max} = maximum growth rate at a particular reference temperature

$f(T)$ = Temperature limiting factor on local growth rate

$f(N)$ = Nutrient limiting factor on local growth rate

$f(I)$ = Light limiting factor on local growth rate

k_z = grazing rate by zooplankton

ω_A = rate of algal settling

6.4 Eutrophication

(1) Temperature limitation

- Three major categories of a temperature adjustment function are used to model algae:

a) Linear function (Bierman et al., 1980; Canale et al., 1975):

$$f(T) = \left(\frac{1}{T_{\text{opt}} - T_{\text{min}}} \right) T - \left(\frac{T_{\text{min}}}{T_{\text{opt}} - T_{\text{min}}} \right) \quad \text{for } T \leq T_{\text{opt}}$$

$$f(T) = 1 \quad \text{for } T > T_{\text{opt}}$$

where

T_{opt} = optimal temperature for algal growth

T_{min} = minimum temperature for algal growth

6.4 Eutrophication

b) Exponential function (Eppley, 1972):

$$f(T) = \theta^{(T-T_{ref})}$$

where

T_{ref} = reference temperature for algal growth (= 20°C)

c) Skewed normal distribution function (Cерco and Cole, 1995):

$$f(T) = \begin{cases} \exp\left[-KTg_1(T_{opt} - T)^2\right], & \text{if } T \leq T_{opt} \\ \exp\left[-KTg_2(T - T_{opt})^2\right], & \text{otherwise} \end{cases}$$

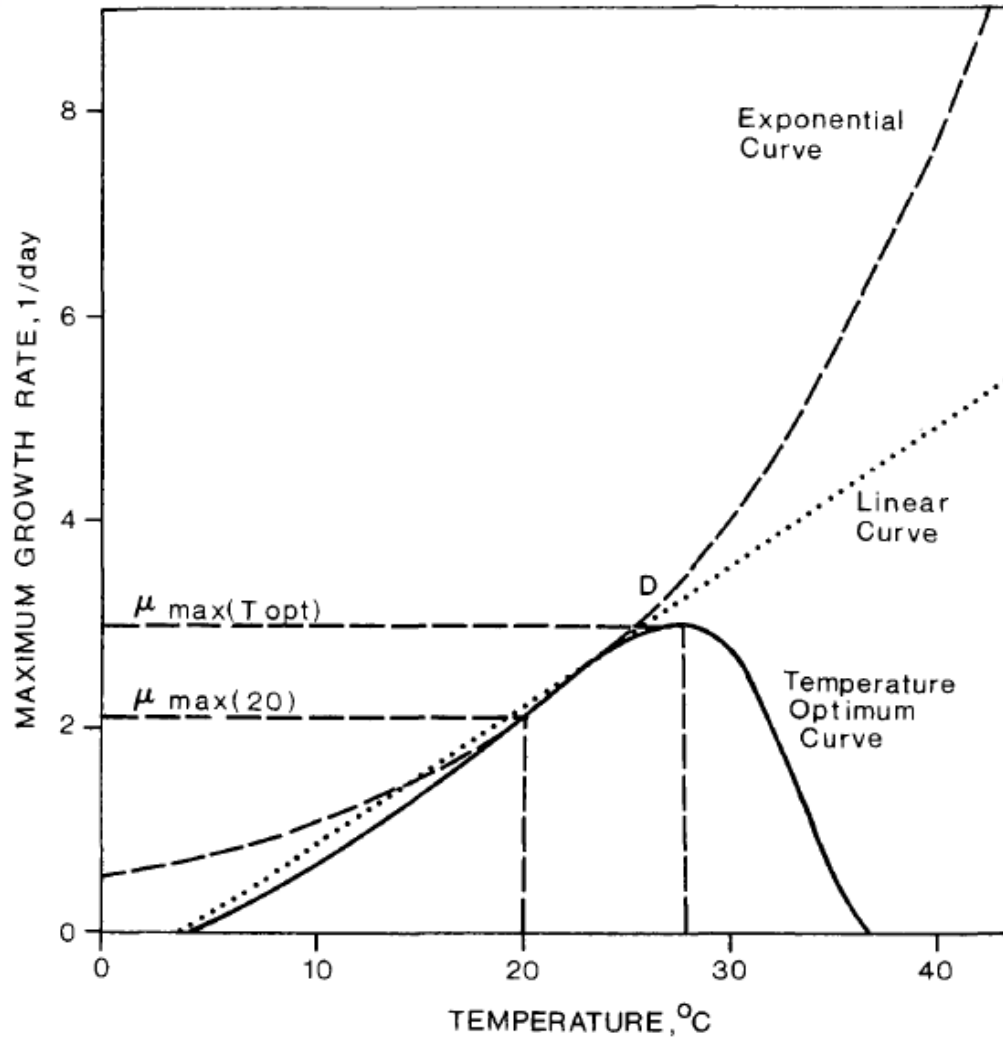
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where

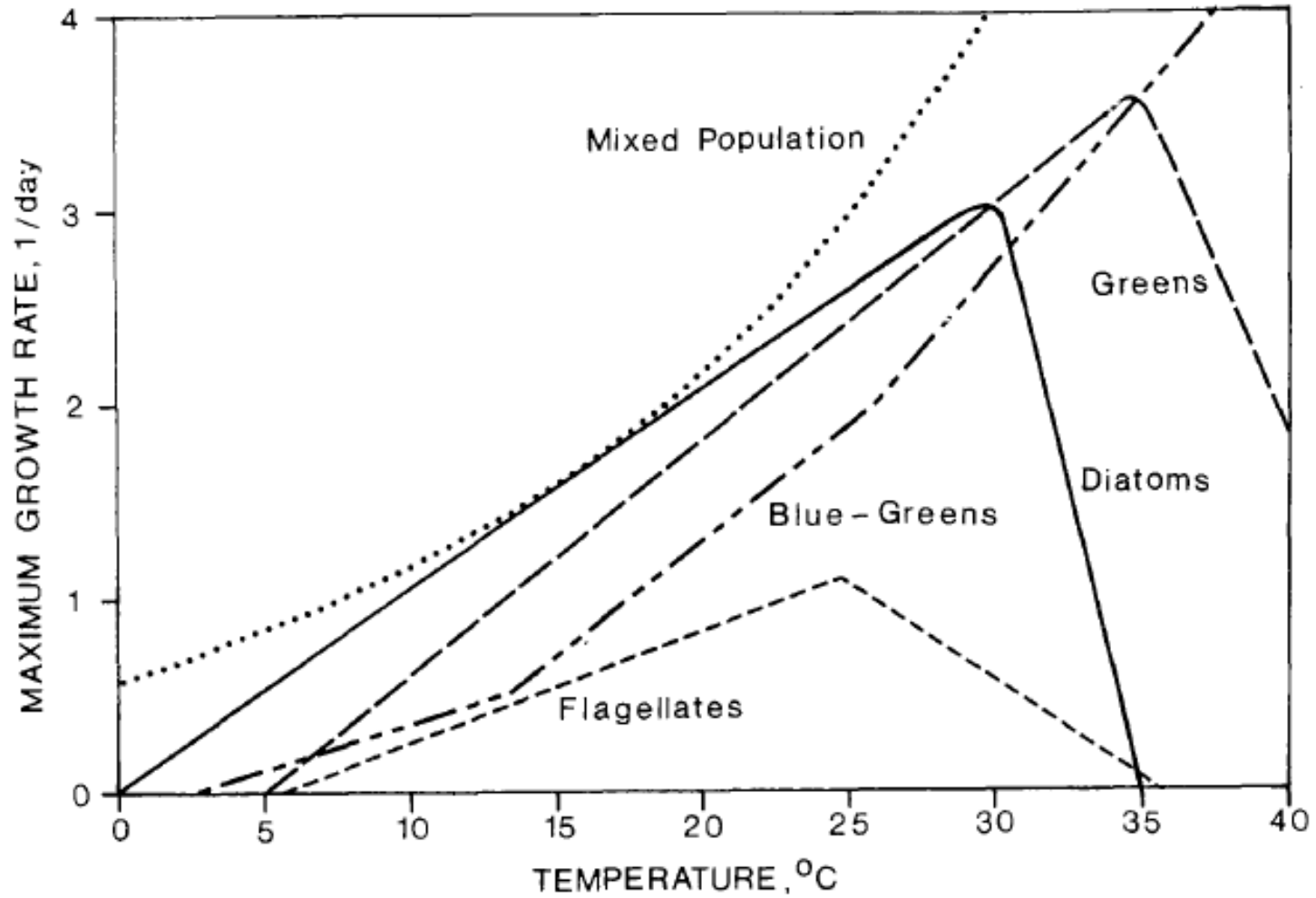
KTg_1 = rate coefficient for left side of curve

KTg_2 = rate coefficient for right side of curve

6.4 Eutrophication



6.4 Eutrophication



6.4 Eutrophication

(2) Nutrient limitation

- Monod model (1945) is frequently used for considering effect of limiting nutrients as substrates on the growth of micro-organisms.

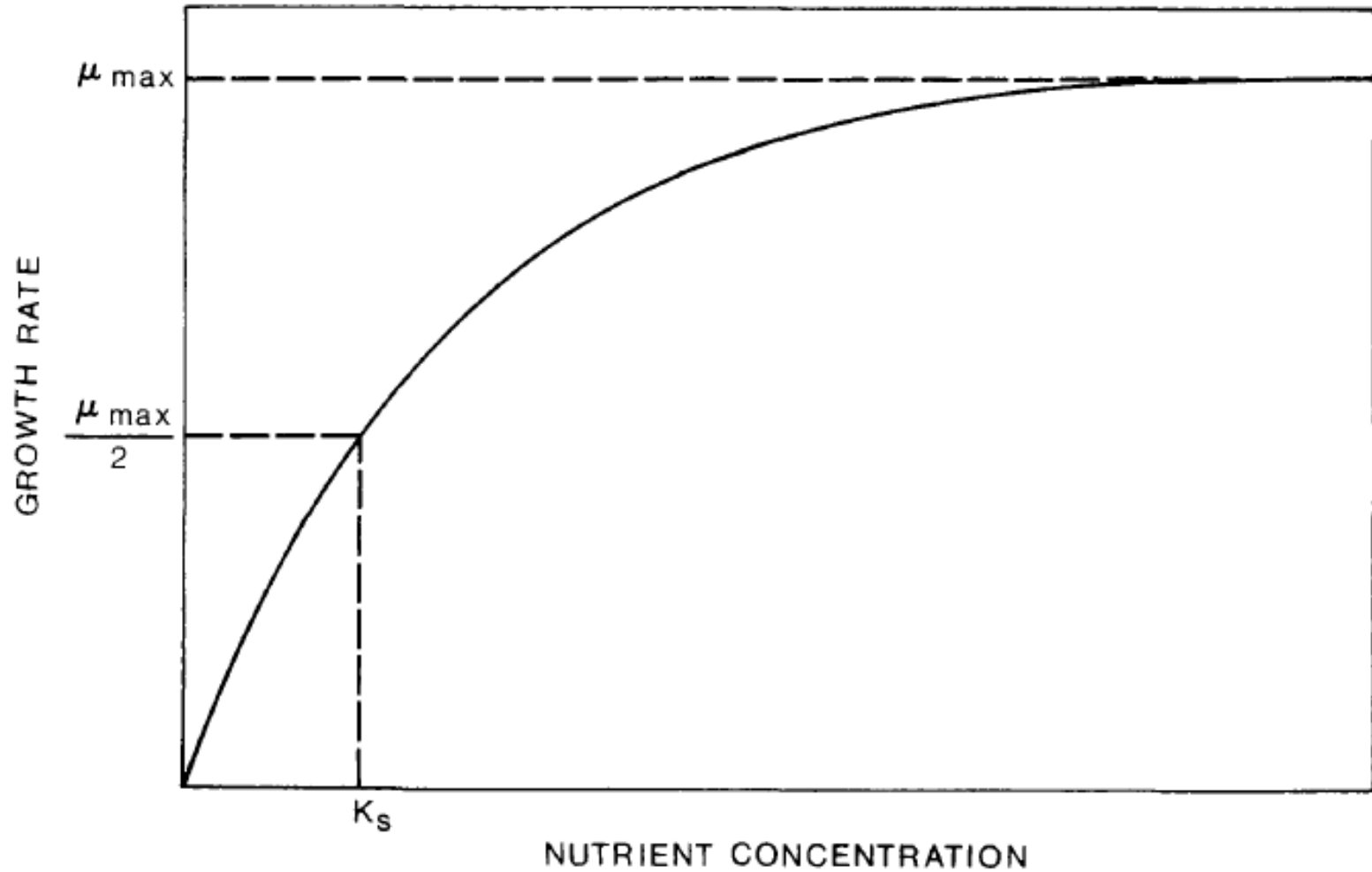
$$\phi_N = \frac{S}{K_S + S}$$

where

S = concentration of the limiting nutrient

K_S = half-saturation constant of the limiting nutrient

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6.4 Eutrophication

- Three primary approaches are used to determine the combined effect of the nutrients:

a) Multiplicative:

$$\phi_N = \frac{N_{nitra}}{K_n + N_{nitra}} \cdot \frac{P_{diss}}{K_p + P_{diss}}$$

b) Limiting nutrient (or Liebig's minimum law):

$$\phi_N = \min \left(\frac{N_{nitra}}{K_n + N_{nitra}}, \frac{P_{diss}}{K_p + P_{diss}} \right)$$

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c) Harmonic mean:

$$\phi_N = \frac{\frac{N_{nitra}}{K_n + N_{nitra}} + \frac{P_{diss}}{K_p + P_{diss}}}{2}$$

where

K_n = half-saturation rate of nitrate nitrogen

K_p = half-saturation rate of phosphate phosphorus

6.4 Eutrophication

(3) Light limitation

- Three formulas are generally used to estimate the light effect on algal growth rate:

a) Michaelis-Menten (saturation) model:

$$\phi_L = \frac{I}{K_{si} + I}$$

b) Steele (photoinhibition) model (1962):

$$\phi_L = \frac{I}{I_S} \cdot e^{1 - \frac{I}{I_S}}$$

6.4 Eutrophication

c) Smith (hyperbolic saturation) model (1936):

$$\phi_L = \frac{I}{\sqrt{I^2 + I_k^2}}$$

where

K_{si} = half-saturation constant of sunlight intensity

I_S = Steele's constant

I_k = Smith's constant

6.4 Eutrophication

