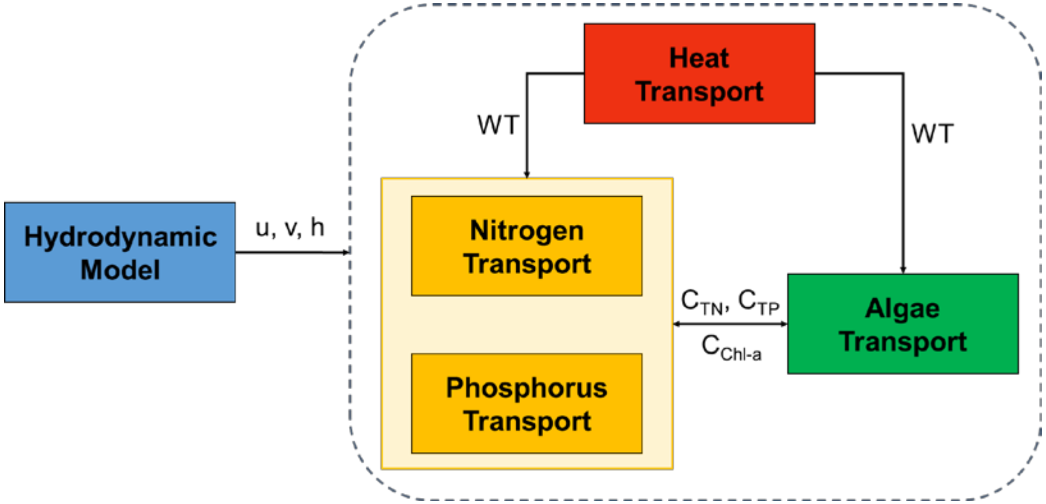
Chapter 6

River Water Quality Modeling



Chapter 6 River Water Quality Modeling

Contents

Objectives

- Classification of non-conservative pollutants
- Present water quality modeling processes

6.1 Non-Conservative Pollutants

6.1.1 Category of Non-Conservative Pollutants

Non-conservative pollutants:

- Substances undergoing any biochemical changes (ex. decay, growth, sink or source) in transport and not following the mass conservation
- Non-conservative pollutants in rivers are generally classified as:

  1) BOD-DO

  2) Heat and temperature

  3) Algae and nutrients

  4) Bacteria and pathogens

  5) Toxic substances

  6) Oil

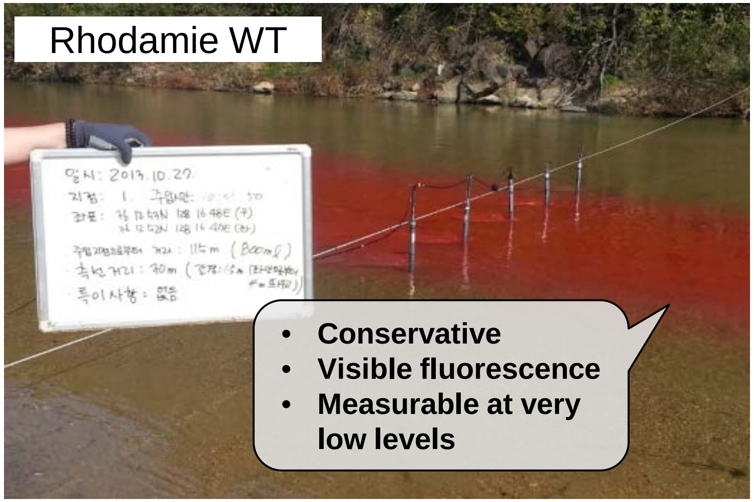
6.1 Non-Conservative Pollutants

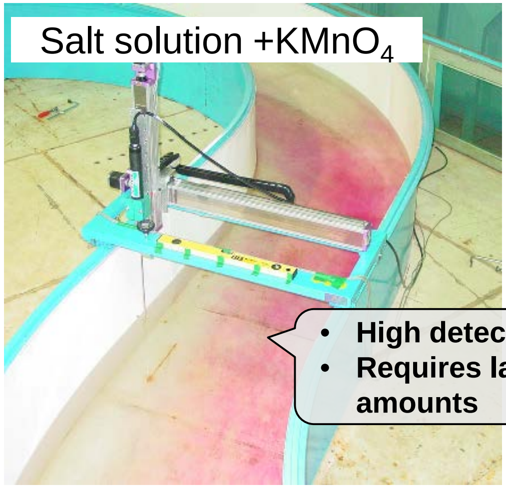
- Toxic substance (독성물질)
  - Metals: mercury, cadmium, lead
  - Industrial chemicals: toluene, benzenes, phenols, PCB
  - Hydrocarbons: PAH (polycyclic aromatic hydrocarbons)
  - Agricultural chemicals: pesticides, herbicides, DDT
  - Radioactive substances

6.1 Non-Conservative Pollutants

[Cf] Conservative pollutants

- One which does not undergo any biochemical changes in transport and follows the mass conservation
- No loss due to chemical reactions or biochemical degradation
- Salt, chloride, total dissolved solids, some metals





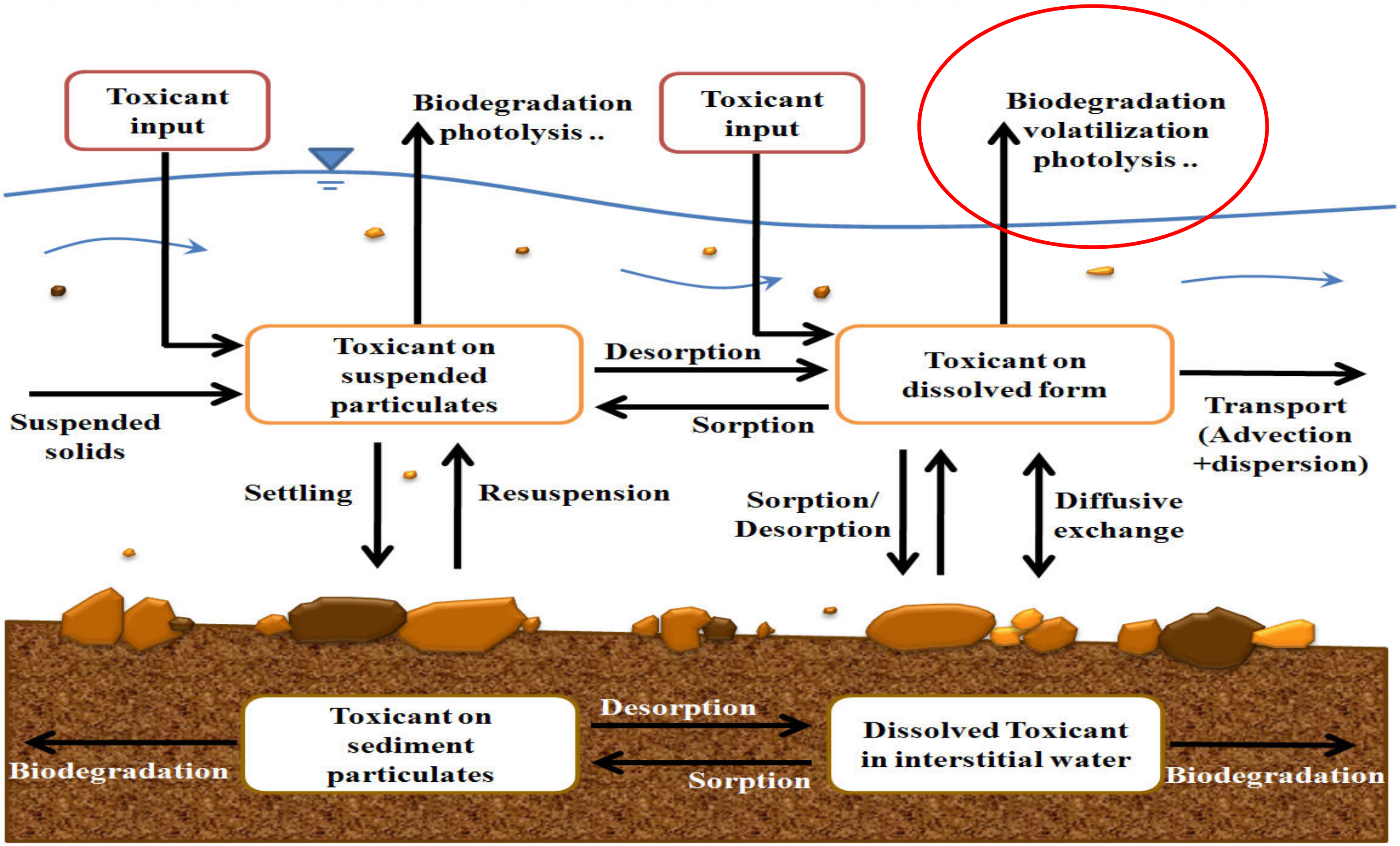
6.1 Non-Conservative Pollutants

6.1.2 Transport of Non-Conservative Pollutants

Physio-chemical phases of the transport of non-conservative substances include

- Loss of the substances 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



6.1 Non-Conservative Pollutants

2D transport model with only loss of the substance

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

where S = sink/source term

Assume first-order decay

- decay rate is proportional to the amount of material present

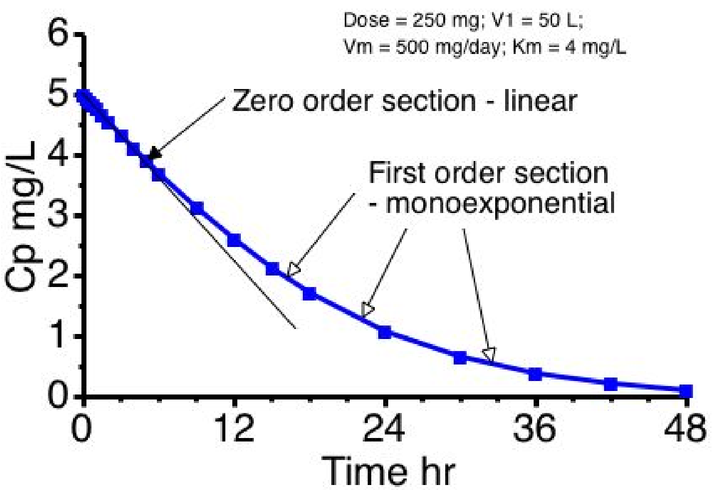
$$\boxed{\frac{dC}{dt}=S=-kC} \Rightarrow \frac{\partial (hC)}{\partial t}+\frac{\partial}{\partial x}(uCh)+\frac{\partial}{\partial y}(vCh)=\nabla\cdot(hD\nabla C)-khC$$

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

6.1 Non-Conservative Pollutants

- First-order decay

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

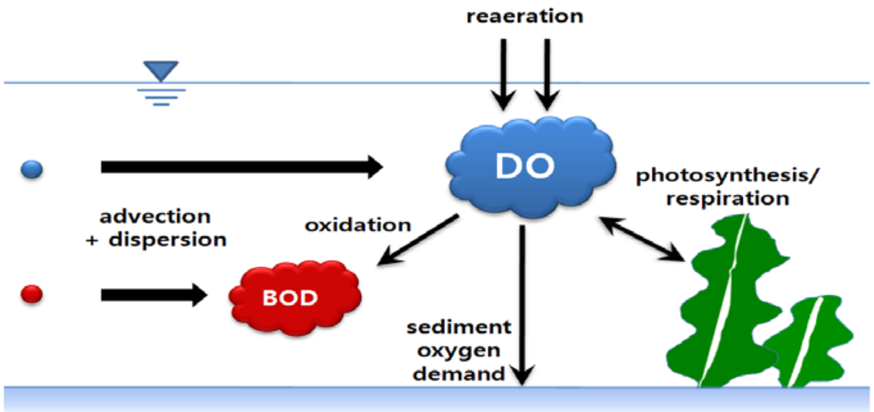


6.2 Modeling BOD-DO Coupled System

6.2.1 Transport of BOD and DO

◆ BOD-DO coupled system

- Conc. of DO depends not only on transport of DO but also on the conc. of BOD present
- Biodegradable substances undergo biochemical reactions
- Oxygen is used up in aerobic decomposition



$$\text{Organic substance} + O_2 \rightarrow CO_2 + H_2O$$

$$\uparrow$$

$$\textit{Bacteria}$$

6.2 Modeling BOD-DO Coupled System

6.2.2 Solutions of BOD-DO Coupled System

◆ Coupled system of BOD and DO

- Determination of DO conc. downstream of a source of BOD

◆ Oxygen Demand (Deoxygenation: 탈산소)

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

- COD: Chemical Oxygen Demand
- BOD: CBOD - Carbonaceous BOD (탄소BOD)

  NBOD – Nitrogeneous BOD(질소BOD)

$$\text{Organic substance} + O_2 \rightarrow CO_2 + H_2O$$

6.2 Modeling BOD-DO Coupled System

◆ Importance of DO

- Anaerobic conditions in a stream are indicative of extreme pollution
- Low DO concentrations have severe effects on aquatic animals

◆ Sources and sinks of DO

Sources	Sinks
- Reaeration from the atmosphere	- Deoxygenation of DO ← BOD
- Photosynthesis oxygen production	- Oxygen demand of sediments of water body
- DO from incoming tributaries	- Use of oxygen for respiration by aquatic plants

$$\therefore \frac{dC}{dt} = \text{reaeration} + (\text{photosynthesis-respiration}) - \text{Deoxygenation by BOD}$$
$$- \text{sediment oxygen demand} \pm \text{oxygen transport (into and out of segment)}$$

6.2 Modeling BOD-DO Coupled System

◆ 1D transport model for BOD and DO

Let C = concentration of DO

L = concentration of BOD

(1) rate of utilization of DO by BOD

$\frac{dL}{dt} = -k_1 L$ → exertion of BOD = utilization of DO = depletion of DO

where k_1 = deoxygenation coefficient (탈산소계수)

∴ Conservation equation for L

$$\boxed{\frac{\partial L}{\partial t} = -U\frac{\partial L}{\partial x} + K\frac{\partial^2 L}{\partial x^2} - k_1 L}$$

⇒ G.E. for BOD

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

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

- 국내 5대강

탈산소계수: 0.05~0.5/day
재폭기계수: 0.25~3.0/day

where k_2 = reaeration coefficient (재폭기계수)

6.2 Modeling BOD-DO Coupled System

∴ Conservation equation for DO

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

Let

$$D = C_s - C$$

Then

$$dD = -dC$$

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

$$\boxed{\frac{\partial D}{\partial t} = -U\frac{\partial D}{\partial x} + K\frac{\partial^2 D}{\partial x^2} + k_1 L - k_2 D}$$

⇒ G.E. for DO Deficit

6.2 Modeling BOD-DO Coupled System

Let reaction terms

$$S_L = -k_r L$$

$$S_D = k_d L - k_a D$$

where

k_r = BOD removal coefficient = $k_d + k_s$

k_s = settling coefficient

k_d = deoxygenation coefficient

k_a = reaeration coefficient

$\therefore$ G.E. for BOD and DOD at unsteady state

BOD $$\frac{\partial L}{\partial t} = -U\frac{\partial L}{\partial x} + K\frac{\partial^2 L}{\partial x^2} - k_r L$$

DOD $$\frac{\partial D}{\partial t} = -U\frac{\partial D}{\partial x} + K\frac{\partial^2 D}{\partial x^2} + k_d L - k_a D$$

6.2 Modeling BOD-DO Coupled System

- *Solution for steady state (continuous input)*

(i) BOD: $0 = -U\dfrac{\partial L}{\partial x} + K\dfrac{\partial^2 L}{\partial x^2} - k_r L$

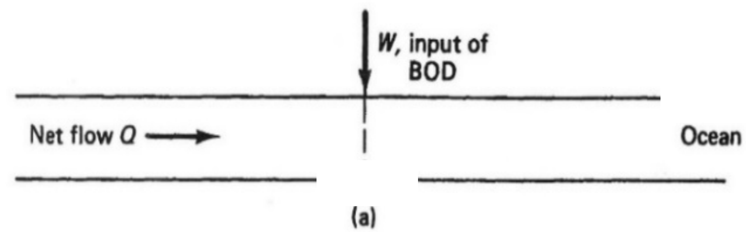
$$L = \begin{bmatrix} L_0 \exp\left[\dfrac{U}{2K}(1+\alpha_r)x\right], & x \le 0 \\ L_0 \exp\left[\dfrac{U}{2K}(1-\alpha_r)x\right], & x \le 0 \end{bmatrix}$$

where

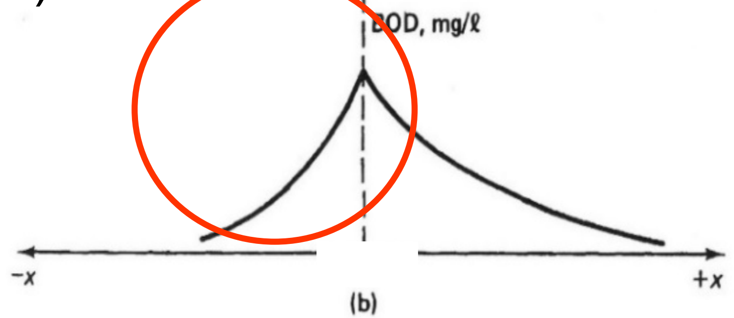
$$L_0 = \frac{W}{Q\alpha_r}$$

$$\alpha_r = \sqrt{1 + \frac{4k_r K}{U^2}}$$

a) input



b) BOD curve



6.2 Modeling BOD-DO Coupled System

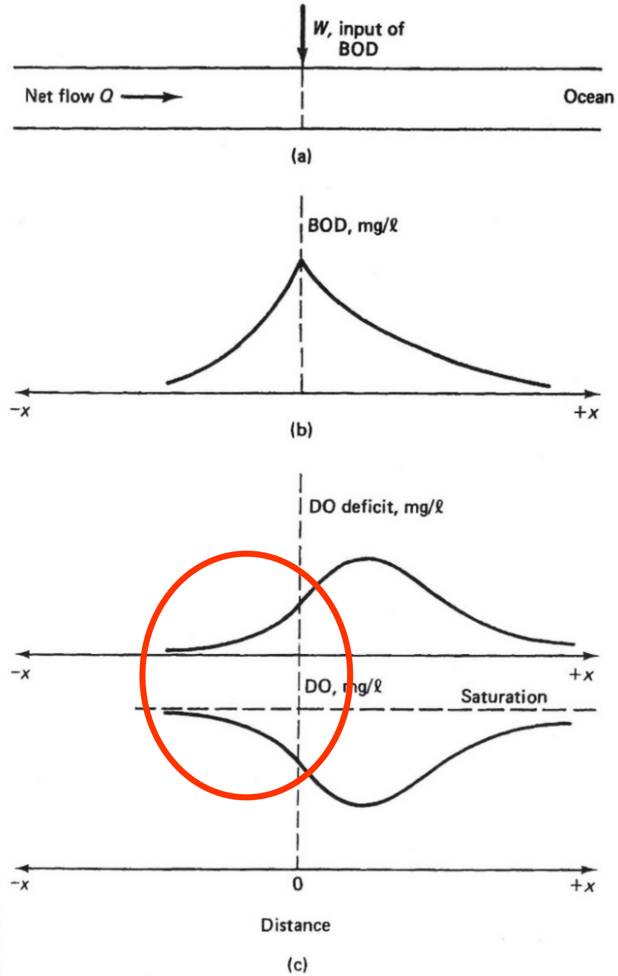
(ii) DO: $$0 = -U\frac{\partial D}{\partial x} + K\frac{\partial^2 D}{\partial x^2} + k_d L - k_a D$$

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

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

where

$$\alpha_a = \sqrt{1 + \frac{4k_a K}{U^2}}$$



6.2 Modeling BOD-DO Coupled System

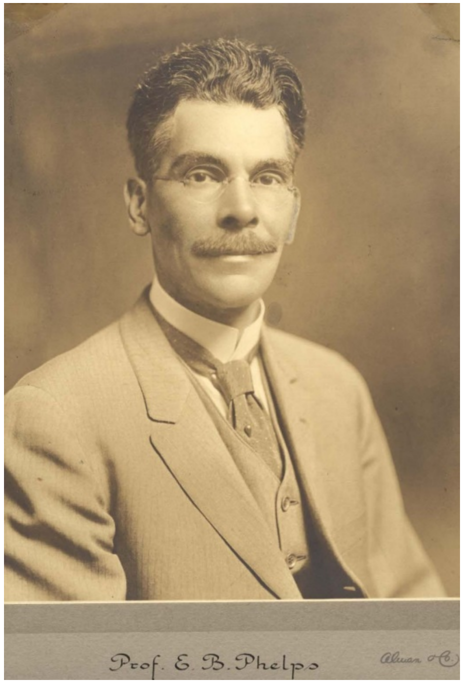
6.2.3 Streeter-Phelps Equation

- Streeter-Phelps Equation (1925)

- No dispersion (river) $K = 0$
- Solution for steady state

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

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 as follow,

$$\boxed{L = L_0 \exp(-\frac{k_1}{U} x) = \frac{W}{Q} \exp(-\frac{k_1}{U} x)}$$

B.C.: $D(0) = D_0 = C_s - C_0$

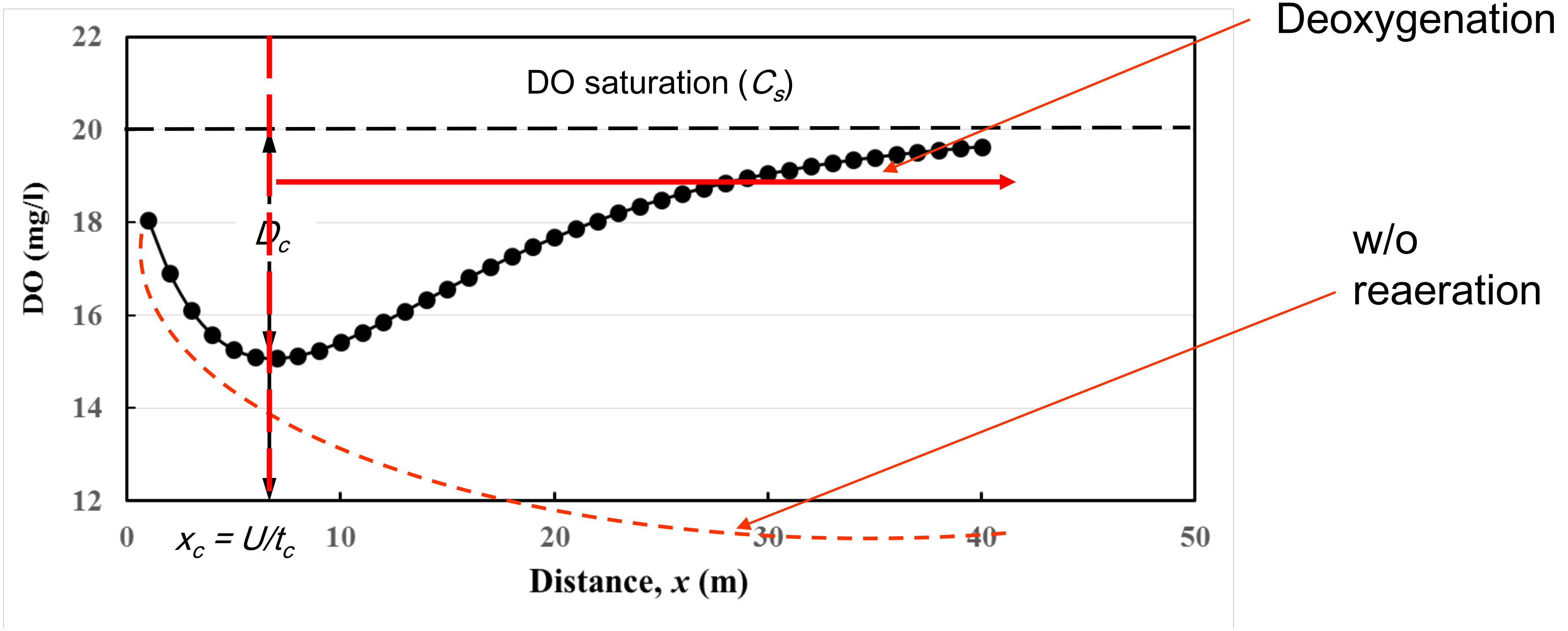
$D_0 = \text{initial deficit}$

Solution:

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

6.2 Modeling BOD-DO Coupled System

◆ DO sag curve



◆ Critical deficit of DO, D_c at t_c

→ Loss of oxygen by BOD balanced by the input of oxygen from atmosphere

6.2 Modeling BOD-DO Coupled System

Change *x* by *t*; *x/U =t* (= time of flow, time of travel)

→ Then Eq. (1) becomes

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

→ t_c may be found as

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

$$\boxed{D_c = \frac{k_1}{k_2} L_0 \, e^{-k_1 t_c}}$$ ← from Eq.(2)

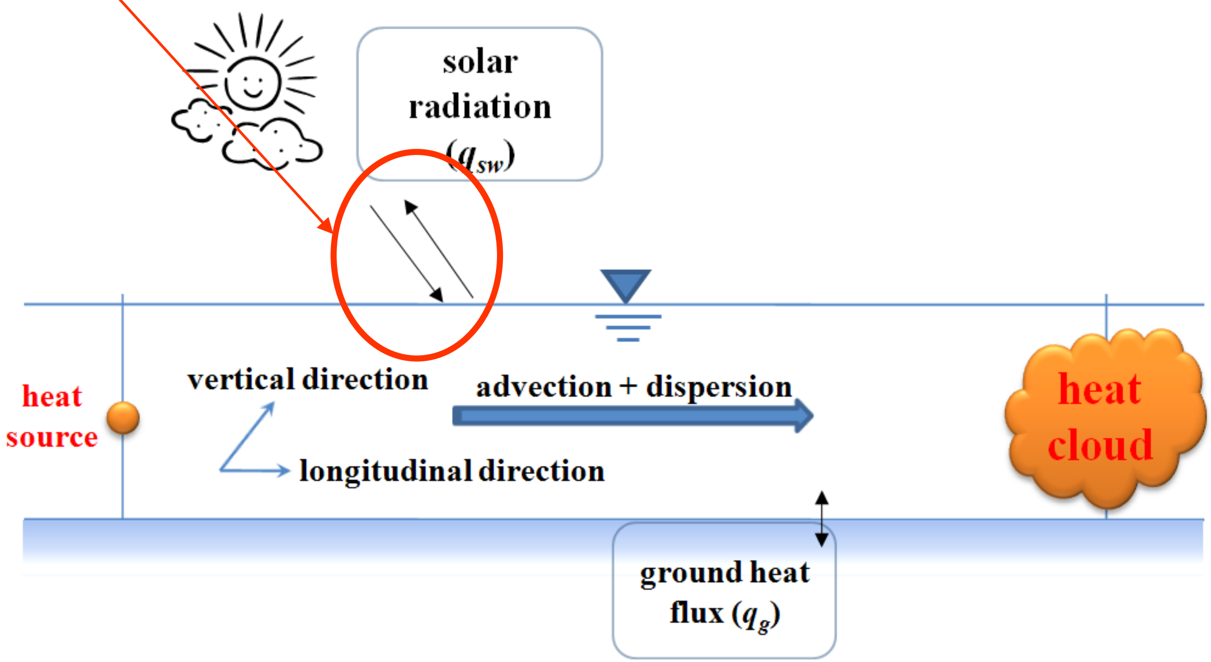
6.3 Modeling Heat Transport

6.3.1 Heat and Water Temperature

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

6.3 Modeling Heat Transport

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



6.3 Modeling Heat Transport

6.3.2 Kinetics of Heat Pollutants

(a) Sources

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

(b) Sinks

- Longwave radiation emitted by water
- Evaporation
- <u>Conduction from water to atmosphere</u>

6.3 Modeling Heat Transport

- Heat balance equation (Edinger & Geyer, 1965; Edinger et al., 1974)

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

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

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

6.3 Modeling Heat Transport

- Simplified heat balance equation

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

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

where

K_T = surface heat exchange coefficient (W/m^2°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_T

- Edinger et al. (1974) proposed as follows,

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

where

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

U_w = wind speed in m/s (at 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 by iteration until q_{net} = 0.
- Alternately, it can be approximated by the empirical relationship as follow,

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

- Time rate of change of temperature

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

where

ρ = water density $(\mathrm{g/cm^3})$

c_p = specific heat of water $(1\ \mathrm{cal/g°C})$

6.3 Modeling Heat Transport

- 2D Heat transport equation

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

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

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

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

6.4 Modeling Eutrophication

6.4.1 Eutrophication

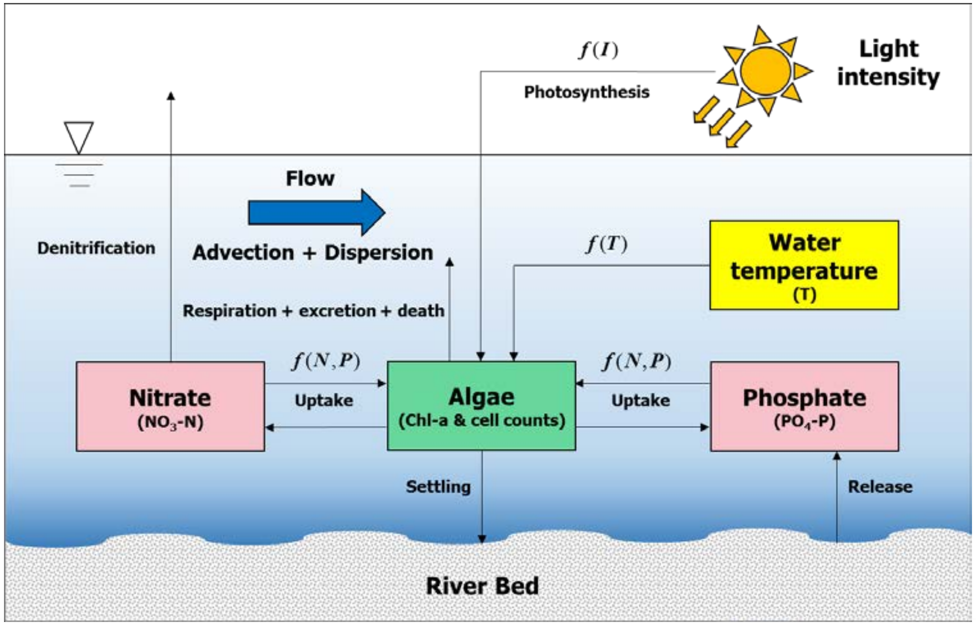
- Eutrophication is excessive nutrient (nitrogen and phosphorus) in the water systems and causes high biomass of algae.
- Toxic algae (cyanobacteria) deteriorates water quality, kills aquatic animals and even damages human organs.

Klamath River, CA

Nakdong River, South Korea

6.4 Modeling Eutrophication

- Nitrogen and phosphorus are crucial proxies to diagnose eutrophication level and calculate growth rate of algae (Thomann & Muller, 1987).
- Algae and nutrients are transported by advection and dispersion with complex physicochemical processes (ex. photosynthesis).



6.4 Modeling Eutrophication

6.4.2 Modeling Nitrogen and Phosphorus

◆ Transport of nitrogen and phosphorus

- Advection and dispersion are the most important mechanisms
- Nutrient transport involves chemical reactions or biological evolutions
- Coupled with algae transport to consider <u>uptake loss by algae</u>
- Also <u>linked with heat transport</u> due to its high influence on nutrient kinetics in the water body

6.4 Modeling Eutrophication

- 1D transport equation of nutrients

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

where

C = concentration of nutrients

K = longitudinal dispersion coefficient

S = sink and source by external contribution

k = first-order decay

Let reaction term of nutrients, $R(C,t) = \pm S - kC$

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

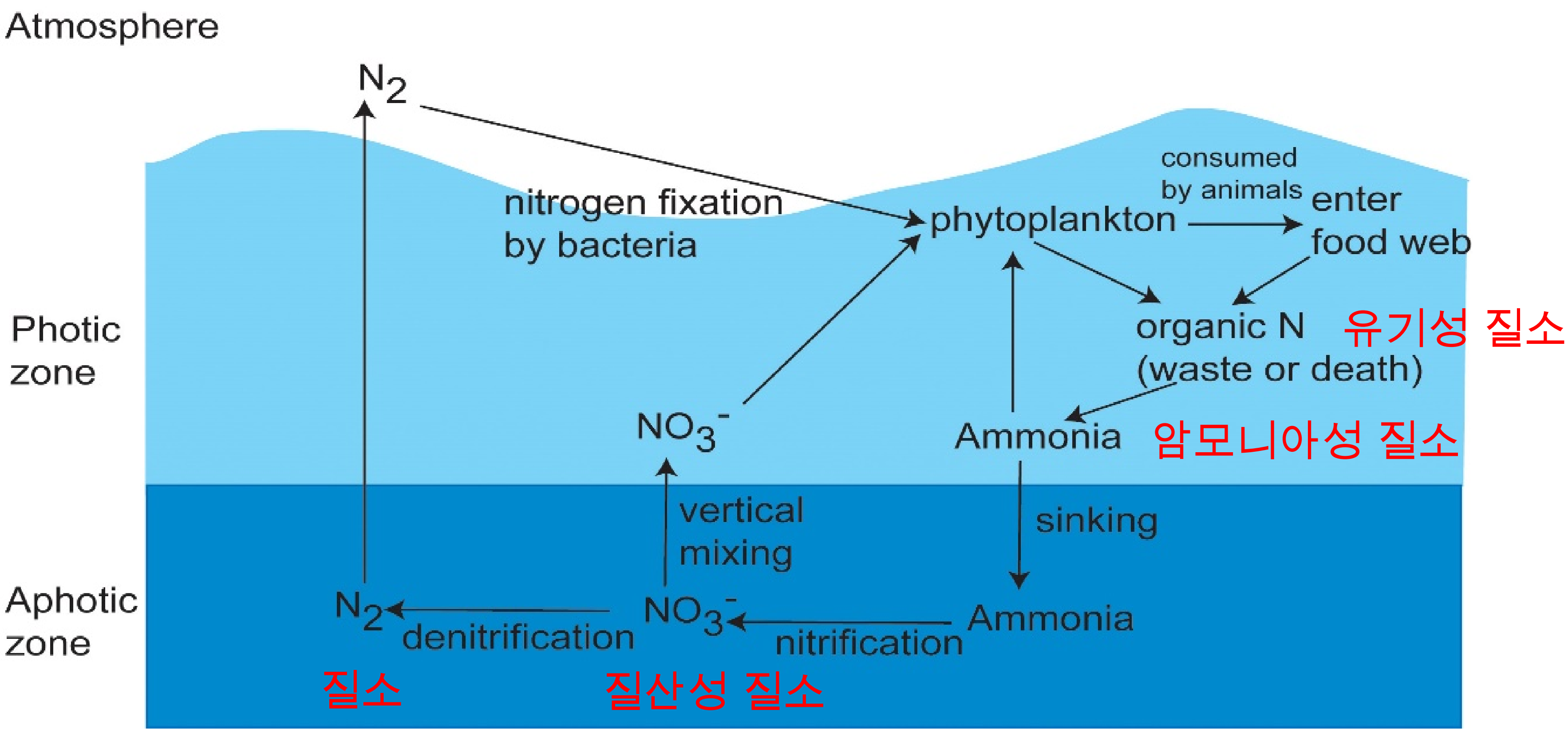
6.4 Modeling Eutrophication

◆ Nitrogen cycle

- Agricultural soil management with synthetic fertilizers, accounts for about 74% of total NO_2 emission in 2013 (USEPA, 2015).
- The nitrogen cycle considers organic nitrogen (Org-N). ammonia nitrogen (NH_4-N), nitrite nitrogen (NO_2-N), and nitrate nitrogen (NO_3-N).
- Nitrification and denitrification are important phases in the nitrogen cycle.

유기성 질소 (Org-N) → 암모니아성 질소 (NH_4-N), → 아질산성 질소 (NO_2-N)
→ 질산성 질소 (NO_3-N)

6.4 Modeling Eutrophication



Source: WATERMAN homepage

6.4 Modeling Eutrophication

- Reaction terms of nitrogen

(1) **Organic nitrogen (Org-N)**

- Source: respiration by algae
- Decay: ammonification from Org-N to ammonia nitrogen, and settling

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

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

where

N_{org} = conc. of organic nitrogen

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

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

θ = temperature coefficient

A = conc. of algae

$k_{n,org}$ = rate of ammonification

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

6.4 Modeling Eutrophication

(2) **Ammonia-nitrogen (NH_4-N)**

- Source: ammonification from organic nitrogen to ammonia-nitrogen
- Decay: nitrification (질화) from ammonia-nitrogen to nitrite-nitrogen

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

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

where

N_{amm} = conc. of ammonia-nitrogen

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

6.4 Modeling Eutrophication

(3) **Nitrite-nitrogen (NO_2-N)**

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

$\therefore R(N_{nitri}, t)$ = nitrification (a) – nitrification (b)

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

where

N_{nitri} = conc. of nitrite-nitrogen

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

6.4 Modeling Eutrophication

(4) **Nitrate-nitrogen (NO_3-N)**

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

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

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

where

N_{nitra} = conc. of nitrate-nitrogen

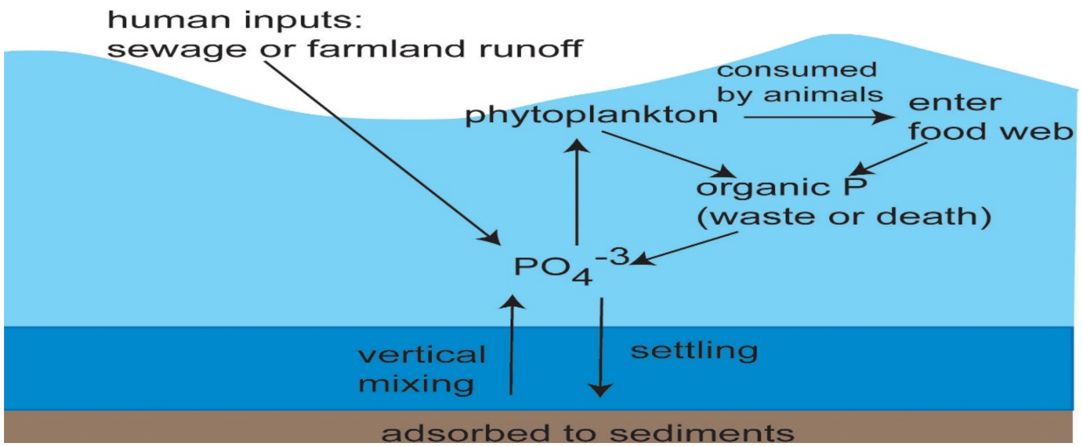
$k_{n,nitra}$ = denitrification rate

μ = algal growth rate

6.4 Modeling Eutrophication

◆ Phosphorus Cycle

- Simpler than the nitrogen cycle with 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).



Source: WATERMAN homepage

6.4 Modeling Eutrophication

◆ Reaction terms of phosphorus

(1) **organic phosphorus (Org-P)**

유기물이 미생물에 의해 무기물로 변화하는 과정

- Source: respiration by algae
- Decay: mineralization (무기화) to phosphate-phosphorus, settling

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

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

where

P_{org} = conc. of organic phosphorus

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

$k_{p,org}$ = mineralization rate

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

6.4 Modeling Eutrophication

(2) **phosphate-phosphorus (PO_4-P)**

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

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

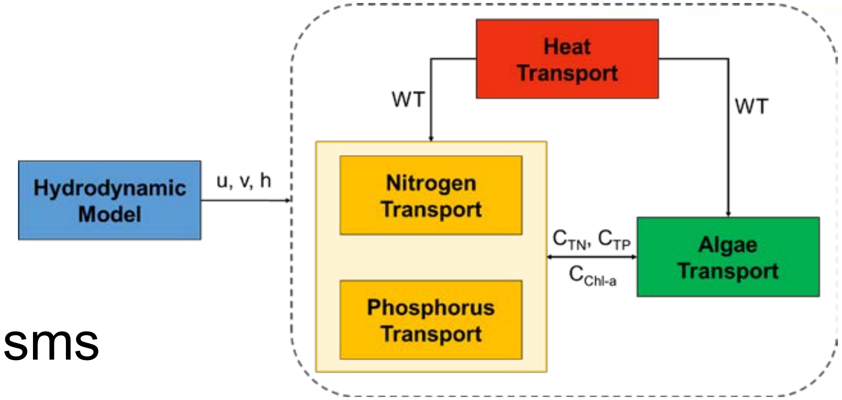
P_{diss} = conc. of phosphate phosphorus

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

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

6.4 Modeling Eutrophication

6.4.3 Modeling Algae



◆ Characteristics of algae

- Aquatic photosynthesis micro-organisms
- Diatom (규조류), green algae and blue-green algae (a.k.a. cyanobacteria) are common species in the water systems
- The presence of algae in the river depends on the factors including: <u>nutrients, temperature, and sunlight intensity </u>(Hornbeger & Kelly, 1975).
- <u>Coupled with nitrogen, phosphorus and heat transport models </u>to estimate growth rate of algae
- <u>Chlorophyll-a (Chl-a) usually used as a proxy of algal </u>concentration

6.4 Modeling 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 1D model:

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

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

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

where

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

6.4 Modeling Eutrophication

◆ Reaction term of algae

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

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

where

$\mu_{\max}$ = maximum growth rate

$f(T)$ = temperature limitation function

$f(N)$ = nutrient limitation function

$f(I)$ = light limitation function

k_z = grazing rate by zooplankton

ω_A = rate of algal settling

6.4 Modeling Eutrophication

(1) **Temperature limitation**

- Three major categories of a temperature limiting function are used to calculate the growth rate of algae:

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

$$f(T) = \begin{cases} \left(\dfrac{1}{T_{opt} - T_{min}}\right) T - \left(\dfrac{T_{min}}{T_{opt} - T_{min}}\right) & , \text{ for } T \le T_{opt} \\ 1 & , \text{ otherwise} \end{cases}$$

where

T_{opt} = optimal temperature for algal growth

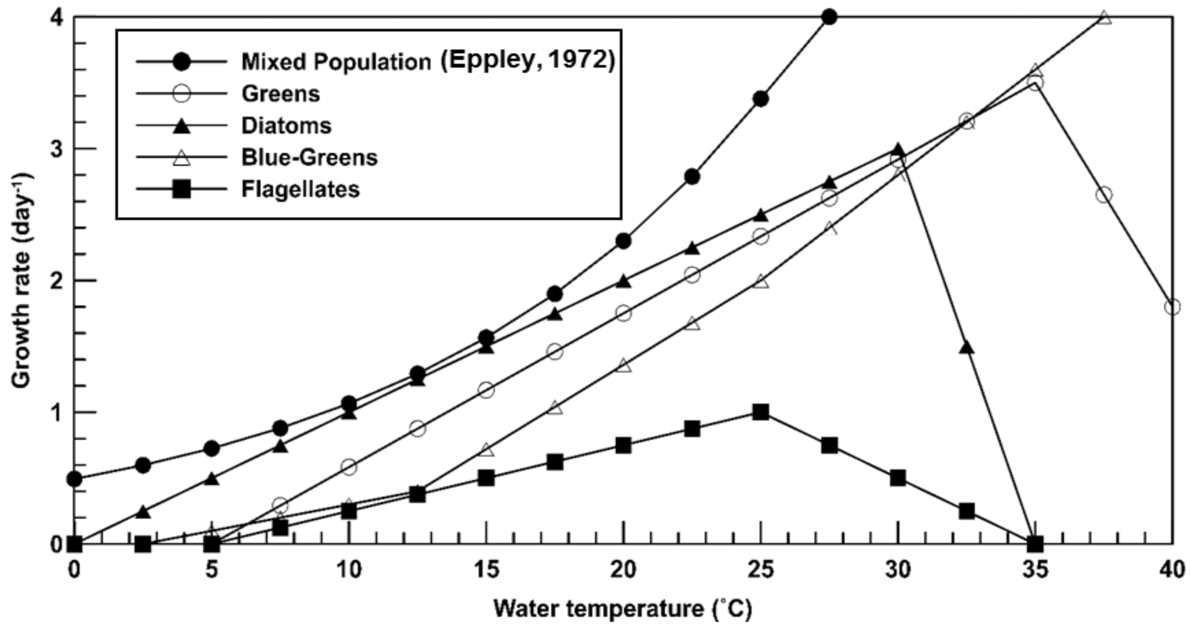
T_{min} = minimum temperature for algal growth

6.4 Modeling Eutrophication

b) Exponential function (Eppley, 1972):

- Can be applied for mixed population of algae in the water body

$f(T) = \theta^{(T - T_{ref})}$ where T_{ref} = reference temperature (= 20˚C)



Source: Canale & Vogel (1974)

6.4 Modeling Eutrophication

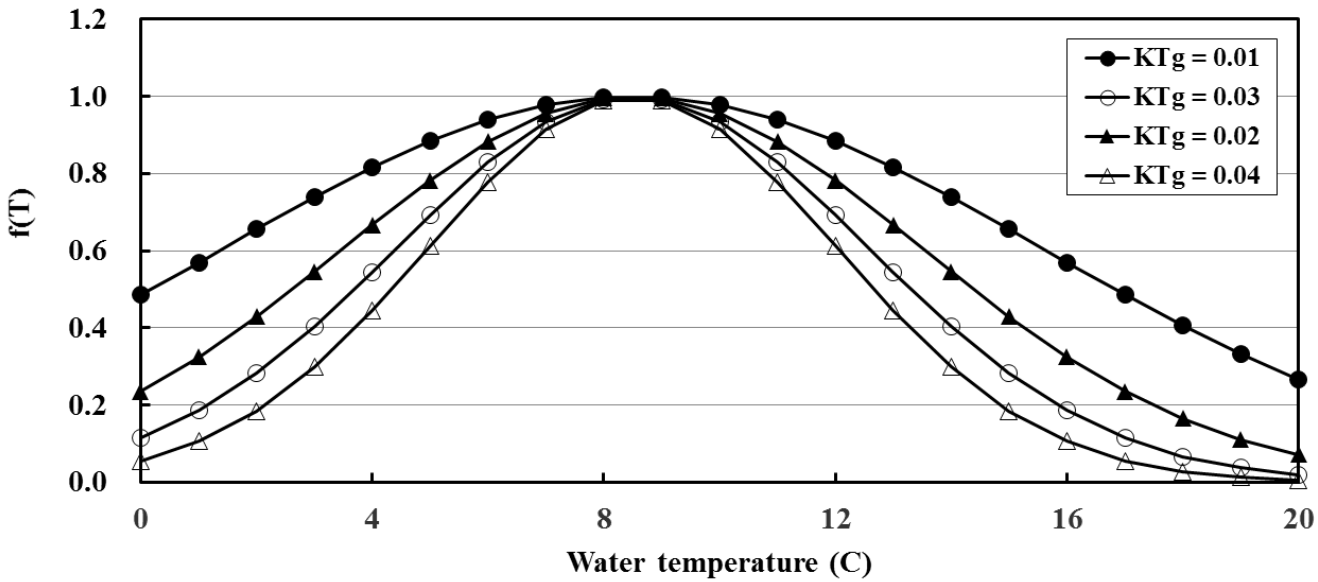
c) Skewed normal distribution function (Cerco & Cole, 1995):

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

where

KTg_1 = rate coefficient for left limb

KTg_2 = rate coefficient for right limb



6.4 Modeling Eutrophication

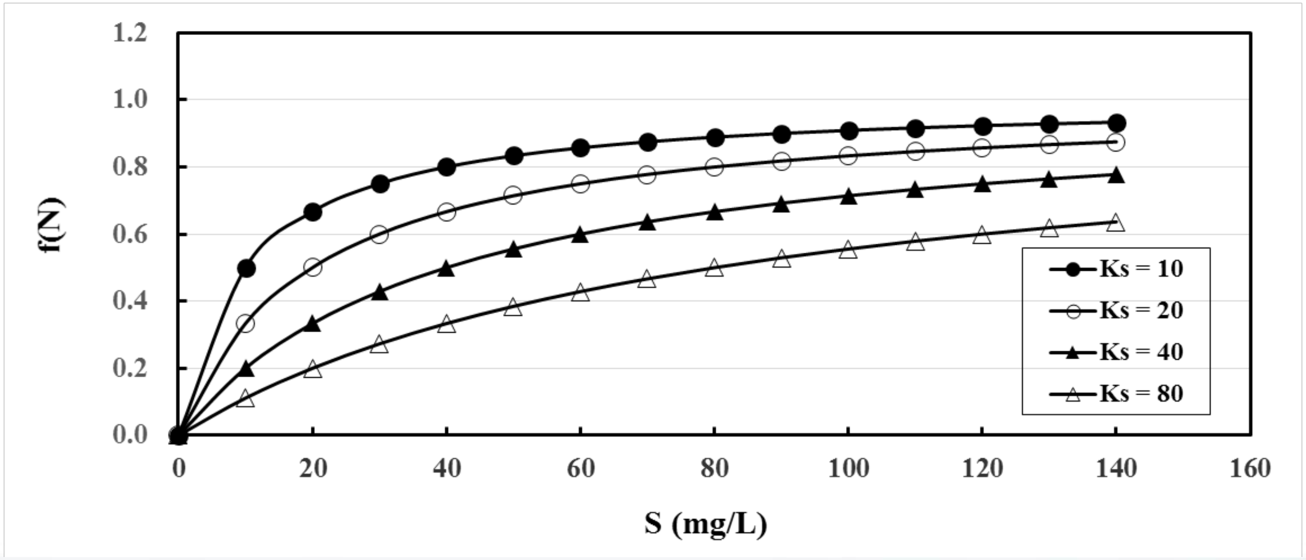
(2) **Nutrient limitation**

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

$$f(N) = \frac{S}{K_S + S}$$ where

S = concentration of the limiting nutrient

K_S = half-saturation constant of the limiting nutrient



6.4 Modeling Eutrophication

- Three approaches used to assess the combined effect of the nutrients:

  a) Multiplicative:

$$f(N) = \frac{N_{nitra}}{K_n + N_{nitra}} \cdot \frac{P_{diss}}{K_p + P_{diss}}$$

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

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

where

K_n = half-saturation rate of nitrogen

K_p = half-saturation rate of phosphorus

  c) Harmonic mean:

$$f(N) = \frac{\frac{N_{nitra}}{K_n + N_{nitra}} + \frac{P_{diss}}{K_p + P_{diss}}}{2}$$

6.4 Modeling Eutrophication

(3) Light limitation

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

a) Michaelis-Menten (saturation) model:

$$f(I) = \frac{I}{K_{si} + I}$$

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

$$f(I) = \frac{I}{\sqrt{I^2 + I_k^{\ 2}}}$$

where

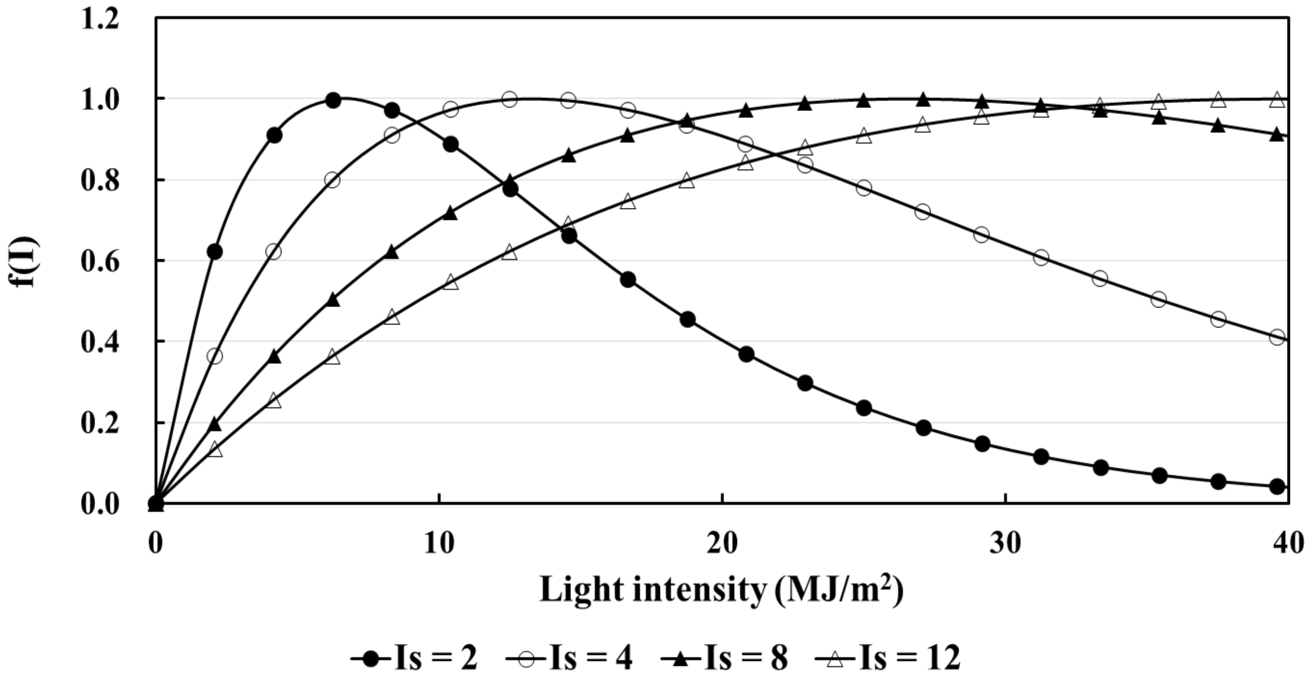
K_{si} = half-saturation constant of sunlight intensity

I_k = Smith's constant

6.4 Modeling Eutrophication

c) Steele (photoinhibition) model (1962):

$$f(I) = \frac{I}{I_S} \cdot e^{1-\frac{I}{I_S}}$$ where I_S = Steele's constant



6.5 Modeling Bacteria and Pathogens

6.5.1 Bacteria and Pathogens

- Cause waterborne diseases (ex. gastroenteritis, amoebasis, cholera, etc.)
- The modes of transmission of pathogens are through drinking water, primary & secondary contact recreation, etc.
- Examples of communicable disease indicators and pathogens

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

6.5 Modeling Bacteria and Pathogens

6.5.2 Kinetics of Bacteria and Pathogens

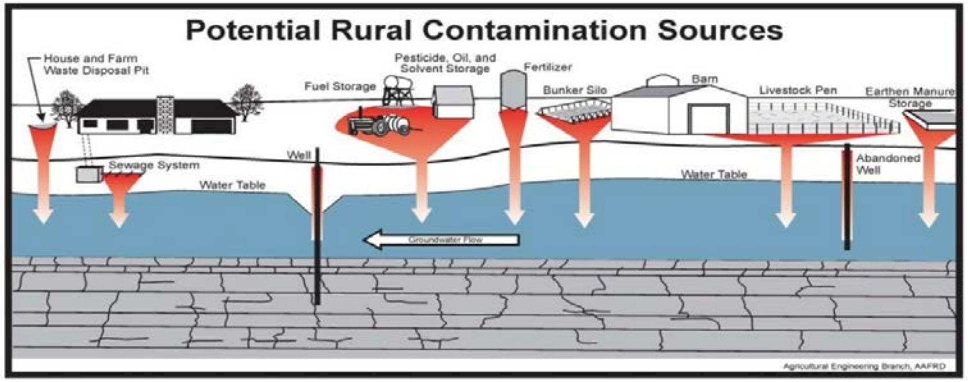
- The principal sources of organisms:

(a) point sources from domestic, municipal, and some industrial sources

(b) combined sewer overflows

(c) runoff from urban and suburban land

(d) municipal waste sludge disposed of on land or in water bodies



Source: Buchanan et al. (2010)

6.5 Modeling Bacteria and Pathogens

- Decay rate of bacteria

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

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

K_{BI} = death rate due to sunlight

K_{Bs} = after growth rate, K_a = net loss due to settling (resuspension)

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

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

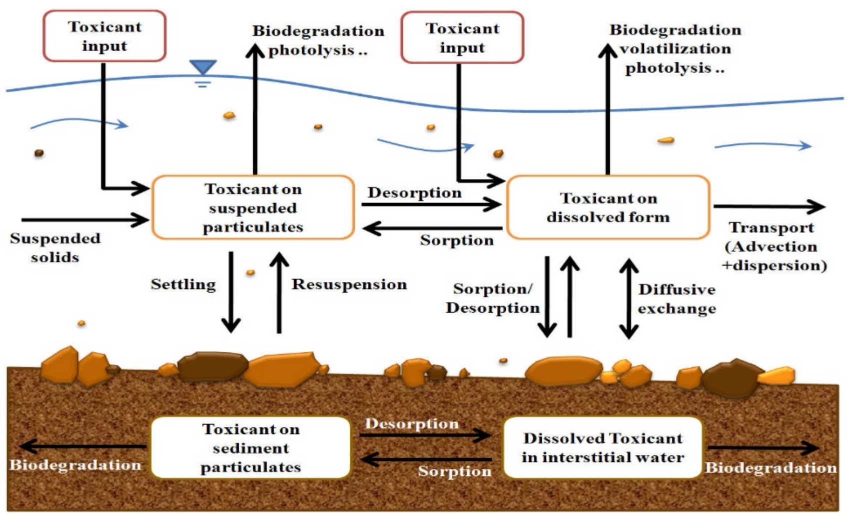
where, N_0 = the concentration at the outfall after mixing [num./L^3],

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

6.6 Modeling Toxic Substances

6.6.1 Kinetics 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
- Settling and resuspension mechanisms of particulates



6.6 Modeling Toxic Substances

2D transport model with 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

$$\frac{dC}{dt} = S = -kC \quad \Rightarrow \quad \frac{\partial (hC)}{\partial t} + \frac{\partial}{\partial x}(uCh) + \frac{\partial}{\partial y}(vCh) = \nabla \cdot (hD\nabla C) - khC$$

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

6.7 Modeling Oil Transport

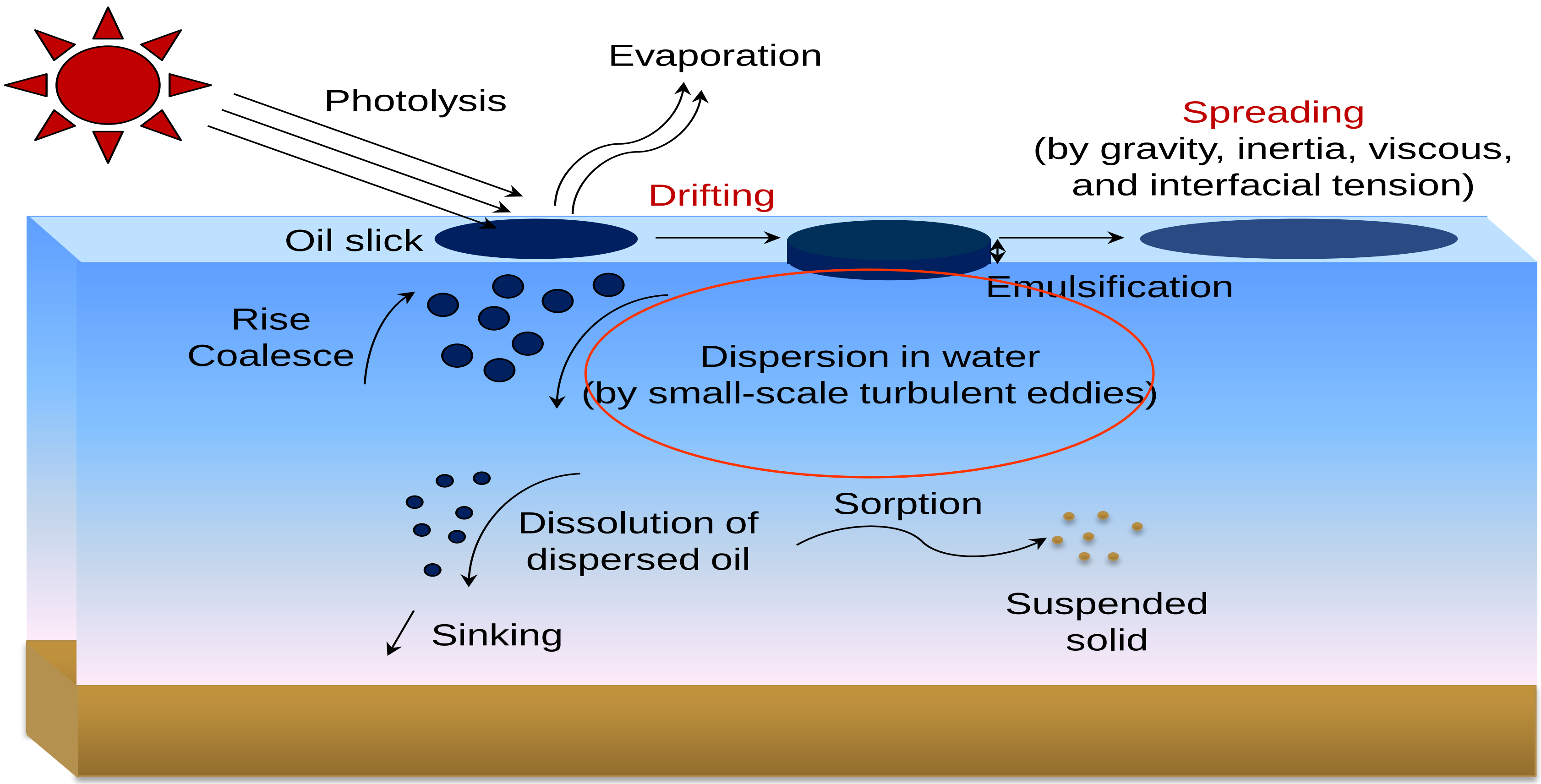
◆ Mechanism of oil transport

- Photolysis (광분해)
- Evaporation
- Advection
- Spreading
- Dispersion
- Sinking

i) Advection

- Advection recognized as a 3-D process with key mechanisms
- <u>Moves horizontally in the water under forcing from wind, wave and current</u>
- <u>Transports vertically in the water column</u> in the form of droplets

6.7 Modeling Oil Transport



6.7 Modeling Oil Transport

ii) Spreading

- Oil film thickness determines the oil persistence on the water surface
- Oil slick area (film thickness) used in the computation of evaporation 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

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

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

6.7 Modeling Oil Transport

iii) Evaporation

- Estimates of evaporative losses are required to assess the spill persistence and the changes in oil properties with time.
- 25 ~ 40% of the total mass can be lost by evaporation, depending on the environmental conditions and the type of oil (Azevedo et al., 2014).
- Evaporative exposure formulation (Stiver & Mackay, 1984)

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

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 from the fractional distillation data

6.7 Modeling Oil Transport

iv) Natural dispersion

- Computation of natural dispersion required for estimate of the spill lifetime
- The rate of natural dispersion depends on environmental parameters and oil parameters (oil film thickness, density, surface tension and viscosity)
- Delvigne & Sweeny (1988) related the number of droplets to the droplet size with a common power law relationship.

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

where $Q_{d \le D}$= 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